Supporting Information

A'-A-π-D-π-A-A' extended small-molecule photovoltaic donor based on fluorene-diketopyrrolopyrrole with end-group fluorination effect

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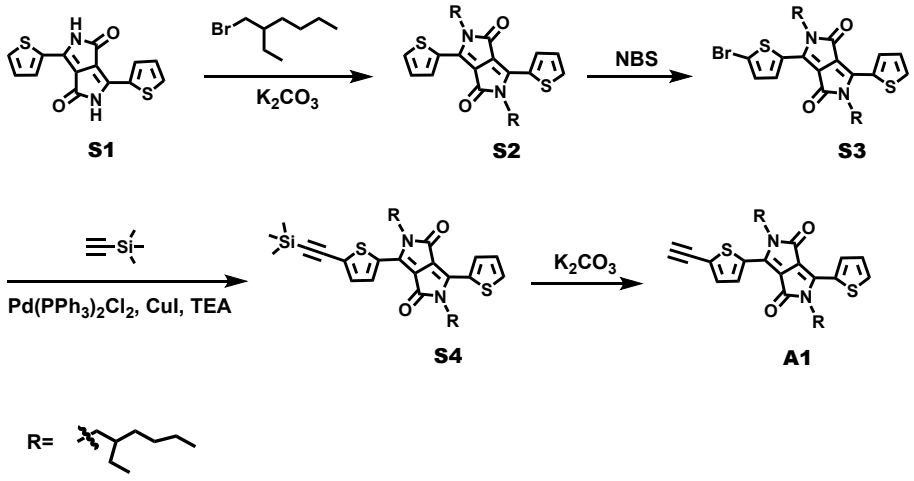
Contents

1. Synthesis



Scheme S1. Synthetic routes of the diketopyrrolopyrrole (DPP)-based compound **A1**.

Synthesis of 3,6-di(thiophen-2-yl)-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (S1)

Compound **S1** was synthesized according to the previously reported methods.[1]

Synthesis of 2,5-bis(2-ethylhexyl)-3,6-di(thiophen-2-yl)-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (S2) [2]

A mixture of compound **S1** (1.80 g, 6 mmol), K_2CO_3 (3.31 g, 24 mmol), 18-crown-6 (0.79 g, 3 mmol), and 35 mL of N, N-dimethylformamide (DMF) was stirred at 120 ℃ for 1 h under nitrogen. Then 1-Bromo-2-ethylhexane (1.73 g, 9 mmol) in DMF (15 mL) was dropped slowly into the reaction solution and heated at 130 ℃ for 18 h under nitrogen. After cooling to room temperature, the mixture was poured into water (50 mL). The resulting mixture was extracted with CH_2Cl_2 (3 × 20 mL) and the combined organic phase was dried over anhydrous Na_2SO_4. After removing the solvent, the residue was purified by column chromatography on silica gel eluting with petroleum ether/CH_2Cl_2 (2:3, v/v) to give a red solid (724 mg, 23%). M.p.: 102-104 °C. ^{1}H-NMR (500 MHz, $CDCl_3$, ppm) δ 8.89 (dd, J_1 = 3.8 Hz, J_2 = 0.9 Hz, 2H), 7.62 (dd, J_1 = 5.0 Hz, J_2 = 0.9 Hz, 2H), 7.27 (d, J = 4.7 Hz, 2H), 4.08-3.97 (m, 4H), 1.91-1.81 (m, 2H), 1.40-1.21 (m,16H), 0.90-0.83 (m, 12H).

Synthesis of 3-(5-bromothiophen-2-yl)-2,5-bis(2-ethylhexyl)-6-(thiophen-2-yl)-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (S3)[3]

A mixture of compound **S2** (840 mg, 1.60 mmol) and $CHCl_3$ (40 mL) was stirred at 0 ℃ for 20 min. A solution of NBS (120 mg, 1.70 mmol) in $CHCl_3$ (10 mL) was added dropwise to the reaction solution at 0 ℃ and the resulting mixture was stirred at room temperature overnight in dark. The reaction solution was poured into water (30 mL) and the resulting solution was extracted with

CH_2Cl_2 (3 × 30 mL). The combined organic phase was dried over anhydrous Na_2SO_4. After removing the solvent, the residue was purified by column chromatography on silica gel with petroleum ether/CH_2Cl_2 (2:3, v/v) as an eluent to afford a red solid. (608 mg, 63%). M.p.:125-127 °C. ^{1}H-NMR (400 MHz, $CDCl_3$, ppm) δ 8.93-8.87 (m, 1H), 8.63 (d, *J* = 4.2 Hz, 1H), 7.69-7.58 (m, 1H), 7.28 (d, *J* = 4.3 Hz, 1H), 7.22 (d, *J* = 4.2 Hz, 1H), 4.04-3.87 (m, 4H), 1.91-1.81 (m, 2H), 1.38-1.21 (m, 16H), 0.92-0.83 (m, 12H).

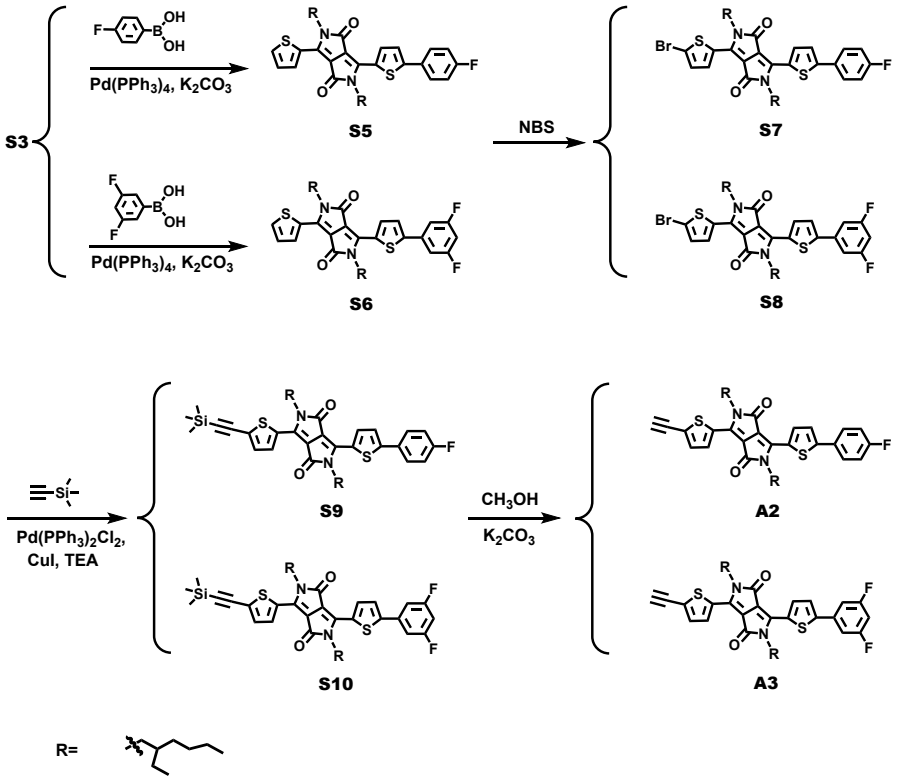
Compound **S4** and **A1** were synthesized by reported procedure.[4] The synthesis details are provided as follows.

Synthesis of 2,5-bis(2-ethylhexyl)-3-(thiophen-2-yl)-6-(5-((trimethylsilyl)ethynyl)thiophen-2-yl)-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (S4)

A mixture of compound **S3** (570 mg, 0.83 mmol), $Pd(PPh_3)Cl_2$ (25 mg, 0.04 mmol), CuI (12 mg, 0.07 mmol), THF (30 mL), TEA (22 mL), and trimethylsilylacetylene (0.4 mL, 2.49 mmol) was heated at 70 °C for 24 h under nitrogen. After cooling to room temperature, the reaction solution was poured into water (30 mL). The resulting solution was extracted with CH_2Cl_2 (3 × 20 mL). The combined organic phase was dried with anhydrous Na_2SO_4. After removing the solvent, the residue was purified by silica gel column chromatography with petroleum ether/CH_2Cl_2 (1:2, v/v) to give a red solid (428 mg, 83%). M.p.:129-131 °C. ^{1}H-NMR (500 MHz, $CDCl_3$, ppm) δ 8.91 (dd, J_1 = 3.9 Hz, J_2 =1.0 Hz, 1H), 8.79 (d, *J* = 4.1 Hz, 1H), 7.64 (dd, J_1 = 5.0 Hz, J_2 = 1.1 Hz, 1H), 7.32 (d, *J* = 4.1Hz, 1H), 7.28-7.27 (m, 1H), 4.07-3.93 (m, 4H), 1.93-1.82 (m, 2H), 1.41-1.22 (m, 16H), 0.92-0.84 (m,12H), 0.28 (s, 9H).

Synthesis of 3-(5-ethynylthiophen-2-yl)-2,5-bis(2-ethylhexyl)-6-(thiophen-2-yl)-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (A1)

A mixture of compound **S4** (428 mg, 0.69 mmol), K_2CO_3 (381 mg, 2.76 mmol), THF (20 mL), and methanol (20 mL) was stirred at room temperature for 2 h. The reaction solution was poured into water (30 mL) and the resulting solution was extracted with CH_2Cl_2 (3 × 20 mL). The combined organic phase was dried with anhydrous Na_2SO_4. After removing the solvent, the residue was purified by silica gel column chromatography with petroleum ether/CH_2Cl_2 (1:2, v/v) to afford a red solid. (356 mg, 94%). M.p.:130-132 °C. ^{1}H-NMR (500 MHz, $CDCl_3$, ppm) δ 8.93 (d, *J* = 3.9 Hz,1H), 8.79 (d, *J* = 4.1 Hz, 1H), 7.65 (d, *J* = 4.9 Hz, 1H), 7.38 (d, *J* = 4.1 Hz, 1H), 7.29-7.26 (m,1H), 4.06-3.94 (m ,4H), 3.58 (s,1H), 1.91-1.83 (m, 2H), 1.38-1.22 (m, 16H), 0.93-0.85 (m,12H).



Scheme S2. Synthetic routes of the diketopyrrolopyrrole (DPP)-based compounds **A2** and **A3**.

Synthesis of 3-(5-(4-fluorophenyl)thiophen-2-yl)-2,5-bis(2-ethylhexyl)-6-(thiophen-2-yl)-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (S5)[5,6]

A mixture of compound **S3** (301 mg, 0.50 mmol), 4-fluorophenylboric acid (105 mg, 0.75 mmol), K_2CO_3 (1.72 g, 12.50 mmol), $Pd(PPh_3)_4$ (22.5 mg, 0.01 mmol), water (6.3 mL), and THF (15 mL) was heated at 80 ℃ for 24 h under nitrogen. After cooling to room temperature, the reaction solution was poured into water (30 mL). The resulting solution was extracted with CH_2Cl_2 (3 × 20 mL). The combined organic phases were dried over anhydrous Na_2SO_4 and then evaporated under reduced pressure. The crude product was purified by column chromatography on silica gel with petroleum ether/CH_2Cl_2 (1:1, v/v) to give a red-purple solid. (294 mg, 95%). M.p.:141-143 °C. ^{1}H-NMR (500 MHz, $CDCl_3$, ppm) δ 8.92 (d, *J* = 4.0 Hz, 1H), 8.89 (d, *J* = 3.5 Hz, 1H), 7.67-7.60 (m, 3H), 7.39 (d, *J* = 4.1 Hz, 1H), 7.27 (d, *J* = 4.2 Hz, 1H), 7.12 (t, *J* = 8.5 Hz, 2H), 4.13-3.96 (m, 4H), 1.98-1.80 (m, 2H), 1.32 (m, 16H), 0.92-0.84(m, 12H).

Synthesis of 3-(5-(3,5-difluorophenyl)thiophen-2-yl)-2,5-bis(2-ethylhexyl)-6-(thiophen-2-yl)-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (S6)[5,6]

A mixture of compound **S3** (277 mg, 0.46 mmol), 3,5-difluoro-phenylboric acid (108 mg, 0.69 mmol), $Pd(PPh_3)_4$ (20 mg, 0.02 mmol), K_2CO_3 (1.58 g, 11.45 mmol), THF (15 mL) and, water (5.8

mL) was heated at 80 ℃ for 24 h under nitrogen. After cooling to room temperature, the reaction solution was poured into water (30 mL). The resulting mixture was extracted with CH_2Cl_2 (3 × 20 mL). The combined organic phase was dried over anhydrous Na_2SO_4. After removing the solvent, the crude product was purified by column chromatography on silica gel with petroleum ether/CH_2Cl_2 (1:1, v/v) to afford a purple-black solid. (286 mg, 98%). M.p.:137-139 °C. ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.93 (dd, J_1 = 4.0 Hz, J_2 = 1.0 Hz, 1H), 8.88 (d, J = 4.1 Hz, 1H), 7.65 (d, J = 5.0 Hz, 1H), 7.46 (d, J = 4.1 Hz, 1H), 7.28 (t, J = 4.0 Hz, 1H), 7.18 (d, J = 6.1 Hz, 2H), 6.83-6.77 (m, 1H), 4.10-3.99 (m, 4H), 1.94-1.83 (m, 2H), 1.43-1.21 (m, 16H), 0.94-0.83 (m, 12H).

Synthesis of 3-(5-bromothiophen-2-yl)-6-(5-(4-fluorophenyl)thiophen-2-yl)-2,5-bis(2-ethylhexyl)-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (S7)[6]

A mixture of compound **S5** (352 mg, 0.57 mmol) and $CHCl_3$ (25 mL)was stirred at 0 ℃ for 20 min. A solution of NBS (101 mg, 0.57 mmol) in $CHCl_3$ (10 mL) was added dropwise to the reaction solution at 0 ℃ and the resulting mixture was stirred at room temperature overnight in dark. The reaction solution was poured into water (30 mL) and the resulting mixture was extracted with CH_2Cl_2 (3 × 20 mL). The combined organic phase was dried over anhydrous Na_2SO_4. After removing the solvent, the crude product was purified by silica gel column chromatography with petroleum ether/CH_2Cl_2 (1:1, v/v) as eluent to give a purple-black solid. (376 mg, 95%). M.p.:147-149 °C. ^{1}H-NMR (500 MHz, $CDCl_3$, ppm) δ 8.93 (d, J = 4.1 Hz, 1H), 8.62 (d, J = 4.2 Hz, 1H), 7.64 (m, 2H), 7.38 (d, J = 4.1 Hz, 1H), 7.21 (d, J = 4.2 Hz, 1H), 7.13 (t, J = 8.5 Hz, 2H), 4.09-3.91 (m, 4H), 1.95-1.81 (m, 2H), 1.43-1.21 (m, 16H), 0.93-0.84 (m,12H).

Synthesis of 3-(5-bromothiophen-2-yl)-6-(5-(3,5-difluorophenyl)thiophen-2-yl)-2,5-bis(2-ethylhexyl)-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (S8)[6]

A mixture of compound **S6** (403 mg, 0.63 mmol) and $CHCl_3$ (25 mL) was stirred at 0 ℃ for 20 min. A solution of NBS (124 mg, 0.70 mmol) in $CHCl_3$ (10 mL) was added dropwise to the reaction solution at 0 ℃ and the resulting mixture was stirred at room temperature overnight in dark. The reaction solution was poured into water (30 mL) and resulting solution was extracted with CH_2Cl_2 (3 × 20 mL). The combined organic phase was dried over anhydrous Na_2SO_4. After removing the solvent, the residue was purified by silica gel column chromatography with petroleum ether/CH_2Cl_2 (1:2, v/v) to give a red solid. (609 mg, 63%). M.p.:177-179 °C. ^{1}H-NMR (500 MHz, $CDCl_3$, ppm) δ 8.89 (d, J = 3.8 Hz, 1H), 8.67 (d, J = 4.0 Hz, 1H), 7.46 (d, J = 4.0 Hz, 1H), 7.23 (d, J =

4.0 Hz, 1H), 7.18 (d, *J* = 6.6 Hz, 2H), 6.81 (t, *J* = 8.7 Hz, 1H), 4.09-3.90 (m, 4H), 1.87 (d, *J* = 5.6 Hz, 2H), 1.44-1.20 (m, 16H), 0.94-0.83 (m, 12H).

The synthesis procedures of compound **S9**, **S10, A2** and **A3** are referred to the reported procedure.[4] The synthesis details are provided as follows.

Synthesis of 3-(5-(4-fluorophenyl)thiophen-2-yl)-2,5-bis(2-ethylhexyl)-6-(5-((trimethylsilyl)ethynyl)thiophen-2-yl)-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (S9)

A mixture of compound **S7** (601 mg, 0.86 mmol), $Pd(PPh_3)_2Cl_2$ (25 mg, 0.04 mmol), CuI (12 mg, 0.07 mmol), THF (25 mL), TEA (22 mL), and trimethylsilylacetylene (0.3 mL, 2.58 mmol) was heated at 70 °C for 24 h under nitrogen. After cooling to room temperature, the reaction solution was poured into water (30 mL). The resulting mixture was extracted with CH_2Cl_2 (3 × 30 mL). The combined organic phase was dried with anhydrous Na_2SO_4. After removing the solvent, the residue was purified by silica gel column chromatography with petroleum ether/CH_2Cl_2 (1:1, v/v) as eluent to afford a purple-black solid. (528 mg, 86%). M.p.:139-141 °C. ^{1}H-NMR (500 MHz, $CDCl_3$, ppm) δ 8.95 (d, *J* = 4.1 Hz, 1H), 8.79 (d, *J* = 4.1 Hz, 1H), 7.68-7.61 (m, 2H), 7.39 (d, *J* = 4.0 Hz, 1H), 7.32 (d, *J* = 4.0 Hz, 1H), 7.13 (t, *J* = 8.4 Hz, 2H), 4.10-3.95 (m, 4H), 1.96-1.83 (m, 2H), 1.42-1.24 (m, 16H), 0.93-0.84 (m, 12H), 0.28 (s, 9H).

Synthesis of 3-(5-(3,5-difluorophenyl)thiophen-2-yl)-2,5-bis(2-ethylhexyl)-6-(5-((trimethylsilyl)ethynyl)thiophen-2-yl)-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (S10)

A mixture of compound **S8** (303 mg, 0.42 mmol), $Pd(PPh_3)_2Cl_2$ (20 mg, 0.03 mmol), CuI (14 mg, 0.07 mmol), THF (20 mL), TEA (11 mL), and trimethylsilylacetyleneto (0.18 mL, 1.26 mmol) was heated at 70 °C for 24 h under nitrogen. After cooling to room temperature, the reaction solution was poured into water (30 mL). The resulting solution was extracted with CH_2Cl_2 (3 × 20 mL). The combined organic layers were dried with anhydrous Na_2SO_4. After removing the solvent, the residue was purified by silica gel column chromatography with petroleum ether/CH_2Cl_2 (1:2, v/v) as eluent to afford a purple-black solid. (276 mg, 89%). M.p.:164-166 °C. ^{1}H-NMR (500 MHz, $CDCl_3$, ppm) δ 8.90 (d, *J* = 4.1 Hz, 1H), 8.82 (d, *J* = 4.1 Hz, 1H), 7.45 (d, *J* = 4.1 Hz, 1H), 7.32 (d, *J* = 4.1 Hz, 1H), 7.18 (d, *J* = 6.1 Hz, 2H), 6.81 (t, *J* = 8.7 Hz, 1H), 4.08-3.96 (m, 4H), 1.94-1.83 (m, 2H), 1.43-1.20 (m, 16H), 0.94-0.84 (m, 12H), 0.28 (s,9H).

Synthesis of 3-(5-ethynylthiophen-2-yl)-6-(5-(4-fluorophenyl)thiophen-2-yl)-2,5-bis(2-ethylhexyl)-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (A2)

A mixture of compound **S9** (614 mg, 0.86 mmol), K_2CO_3 (1.58 g, 11.45 mmol), THF (25 mL), and methanol (25 mL) was stirred at room temperature for 2 h. The reaction solution was poured into water (30 mL) and the resulting solution was extracted with CH_2Cl_2 (3 × 20 mL). The combined organic was dried with anhydrous Na_2SO_4. After removing the solvent, the residue was purified by silica gel column chromatography with petroleum ether/CH_2Cl_2 (1:1, v/v) to afford a black solid. (408 mg, 74%). M.p.:133-135 °C. ^{1}H-NMR (500 MHz, $CDCl_3$, ppm) δ 8.96 (d, *J* = 4.1 Hz,1H), 8.79 (d, *J* = 4.1 Hz, 1H), 7.65 (dd, J_1 = 8.2 Hz, J_2 = 5.3 Hz, 2H), 7.41-7.36 (m, 2H), 7.13 (t, *J* = 8.6 Hz, 2H), 4.10-3.94 (m, 4H), 3.58 (s, 1H), 1.96-1.84 (m, 2H), 1.37-1.25 (m, 16H), 0.92-0.85 (m,12H).

Synthesis of 3-(5-(3,5-difluorophenyl)thiophen-2-yl)-6-(5-ethynylthiophen-2-yl)-2,5-bis(2-ethyl hexyl)-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (A3)

A mixture of compound **S10** (276 mg, 0.38 mmol), K_2CO_3 (212 mg, 1.52 mmol), THF (15 mL), and methanol (15 mL) was stirred at room temperature for 2 h. The reaction solution was poured into water (30 mL) and the resulting solution was extracted with CH_2Cl_2 (3 × 20 mL). The combined organic phase was dried with anhydrous Na_2SO_4. After removing the solvent, the residue was purified by silica gel column chromatography with petroleum ether/CH_2Cl_2 (1:2, v/v) to give a black solid. (156 mg, 62%). M.p.:154-156 °C. ^{1}H-NMR (500 MHz, $CDCl_3$, ppm) δ 8.93 (d, *J* = 4.1 Hz, 1H), 8.83 (d, *J* = 4.1 Hz, 1H), 7.46 (d, *J* = 4.1 Hz, 1H), 7.38 (d, *J* = 4.1 Hz, 1H), 7.18 (d, *J* = 6.1 Hz, 2H), 6.85-6.78 (m, 1H), 4.10-3.95 (m, 4H), 3.59 (s, 1H), 1.94-1.83 (m, 2H), 1.33-1.18 (m, 16H), 0.93-0.81 (m, 12H).

2. Spectra of ^{1}H-NMR, ^{13}C-NMR, and MALDI-TOF HRMS

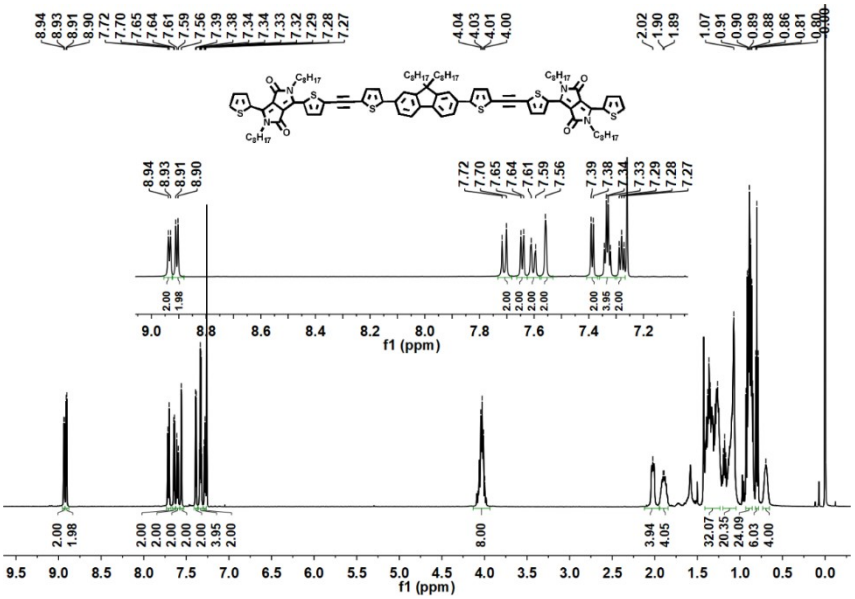


Figure S1. ^{1}H-NMR spectrum of **Flu(DPP)$_2$**.

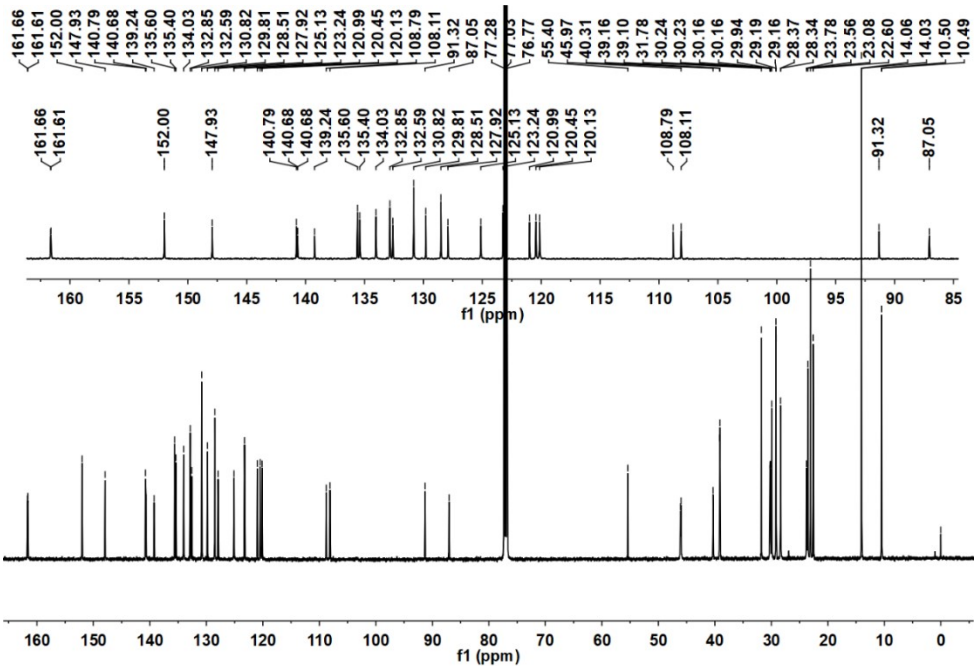


Figure S2. ^{13}C-NMR spectrum of **Flu(DPP)$_2$**.

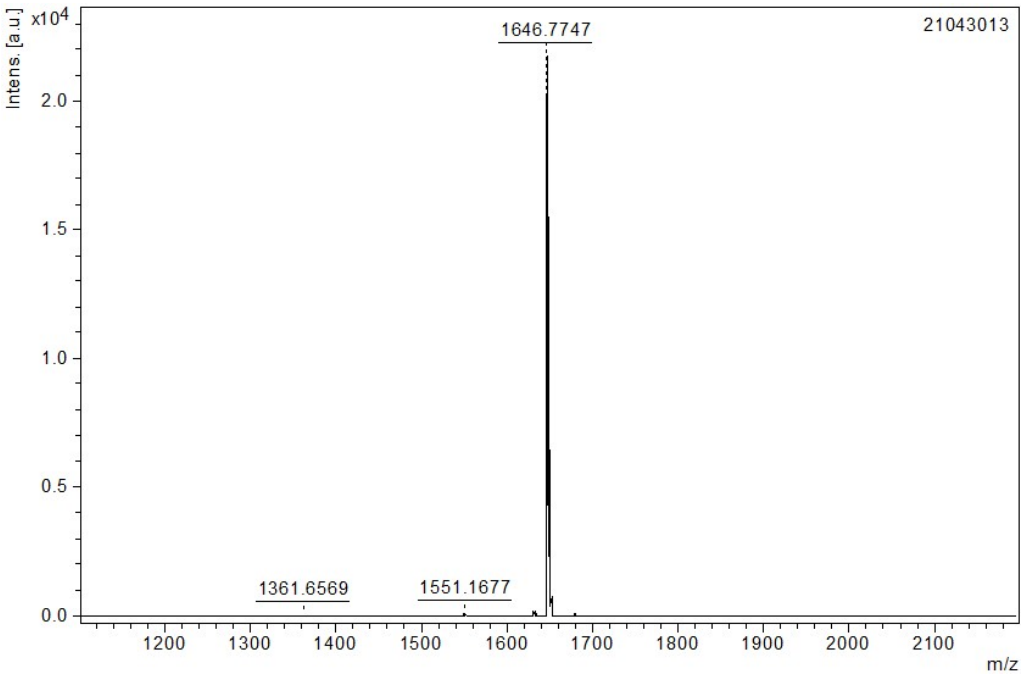


Figure S3. MALDI-TOF HRMS spectrum of **Flu(DPP)$_2$**. (calcd for $C_{101}H_{122}N_4O_4S_6$：1646.7990)

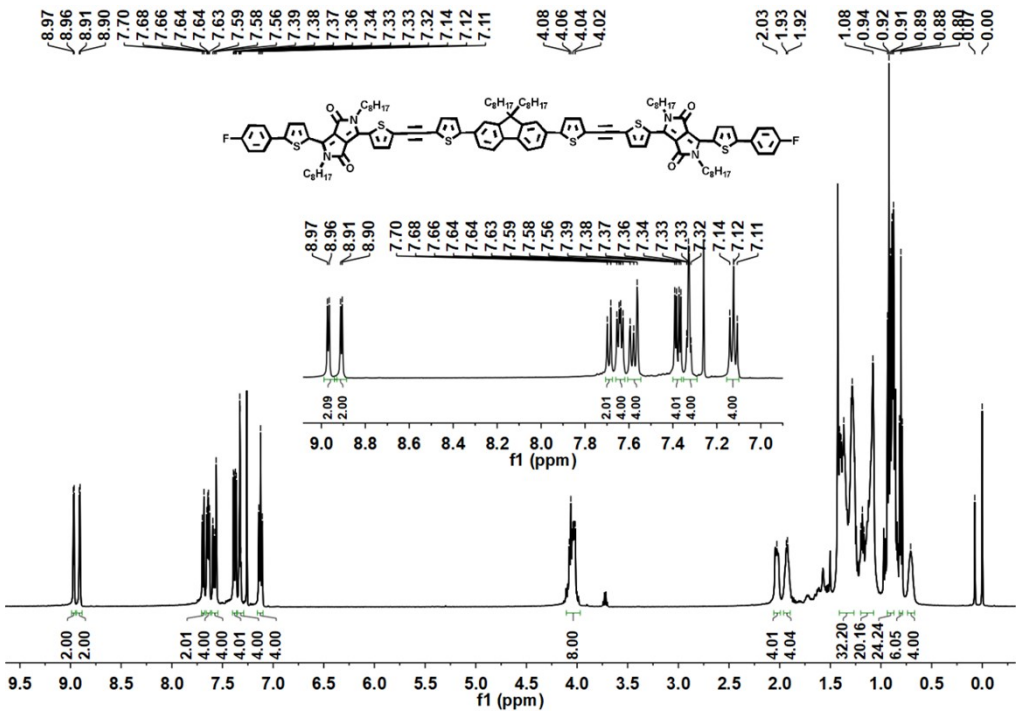


Figure S4. ^{1}H-NMR spectrum of **Flu(DPPsF)$_2$**.

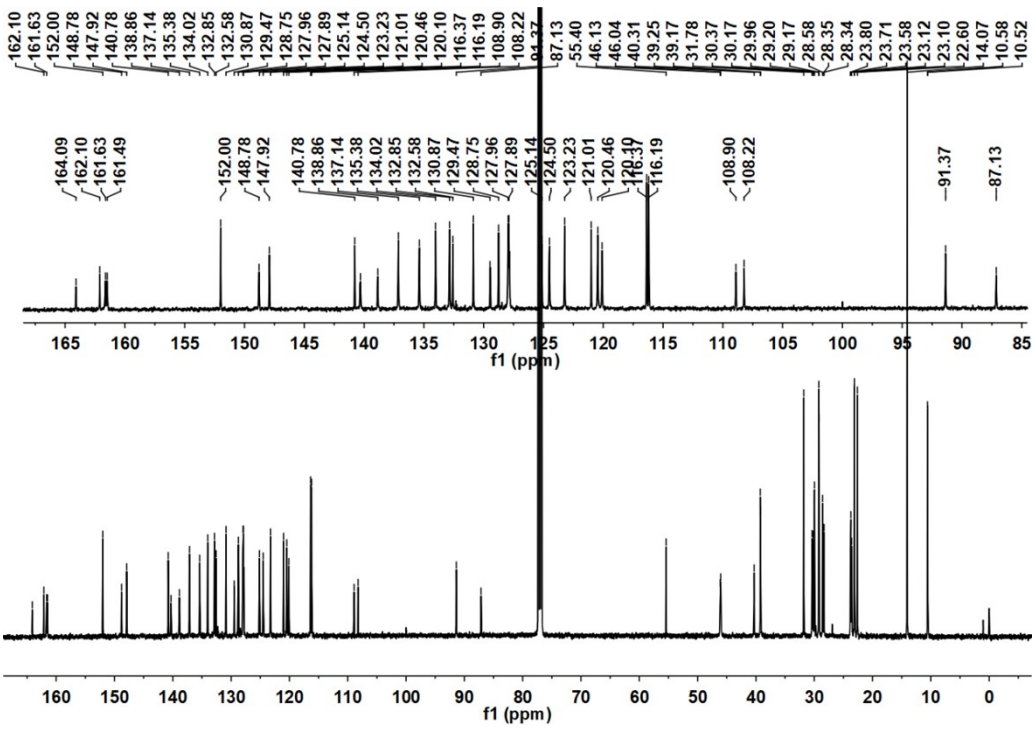


Figure S5. ^{13}C-NMR spectrum of **Flu(DPPsF)$_2$**.

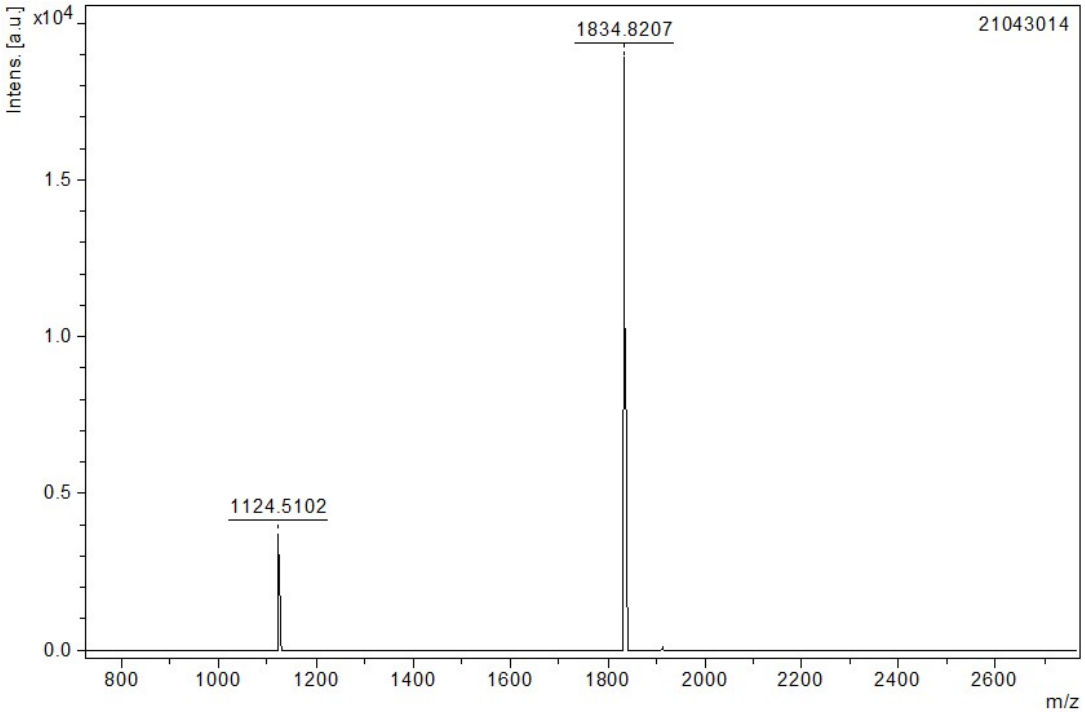


Figure S6. MALDI-TOF HRMS spectrum of **Flu(DPPsF)$_2$**. (calcd for $C_{113}H_{128}F_2N_4O_4S_6$：1834.8228)

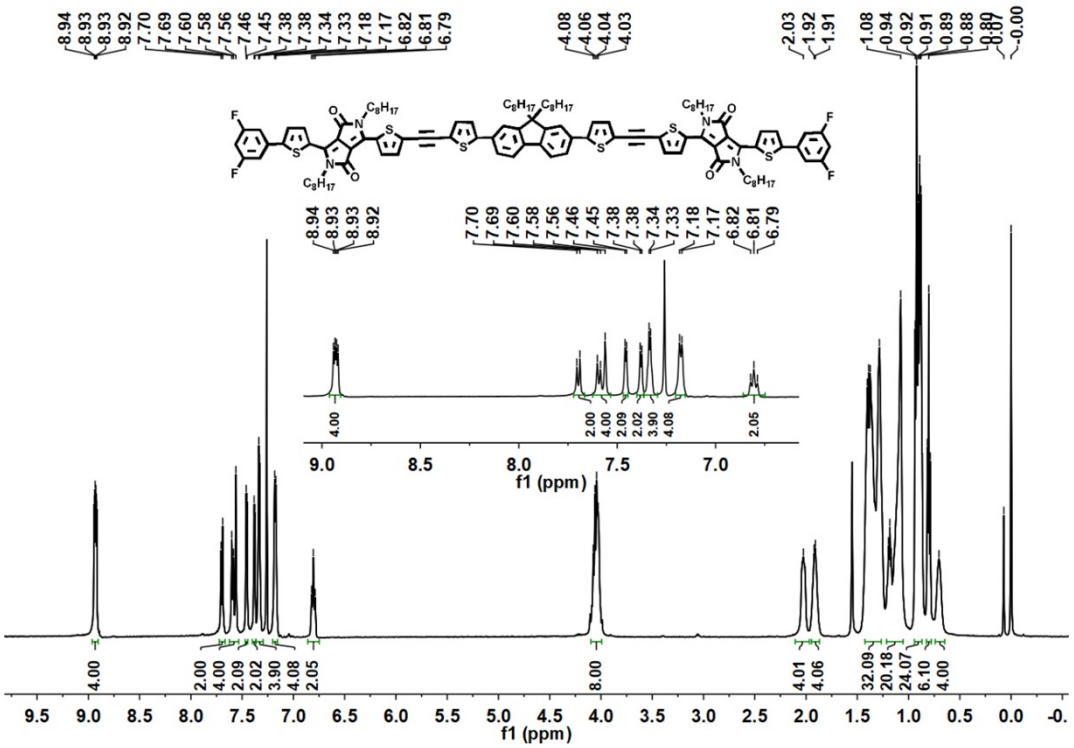


Figure S7. ^{1}H-NMR spectrum of **Flu(DPPdF)$_2$**.

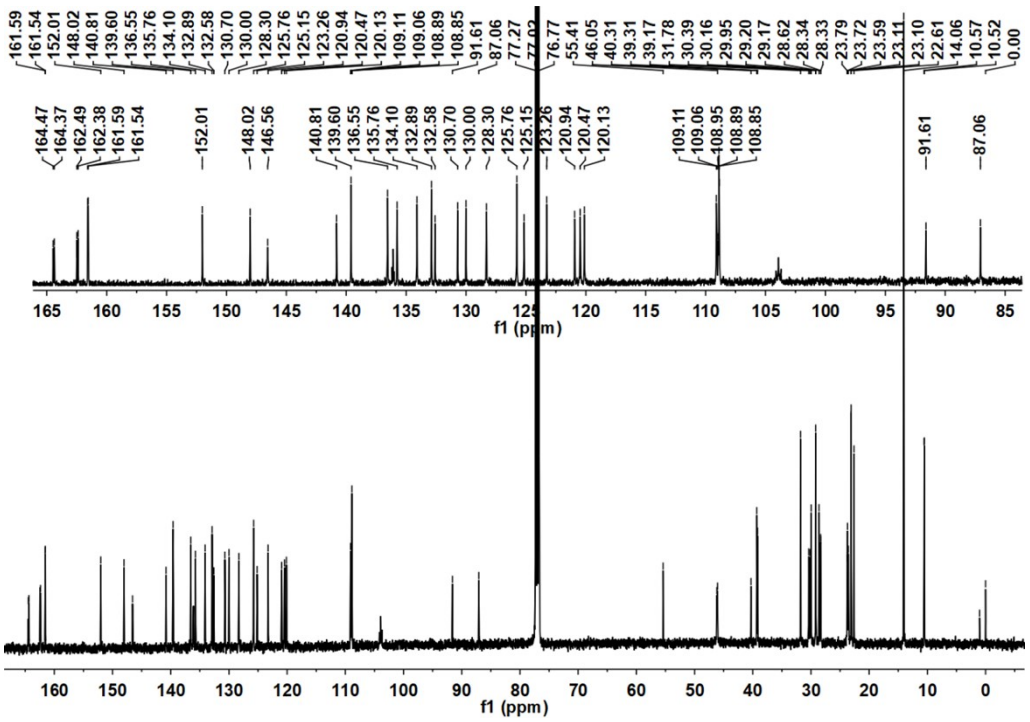


Figure S8. ^{13}C-NMR spectrum of **Flu(DPPdF)$_2$**.

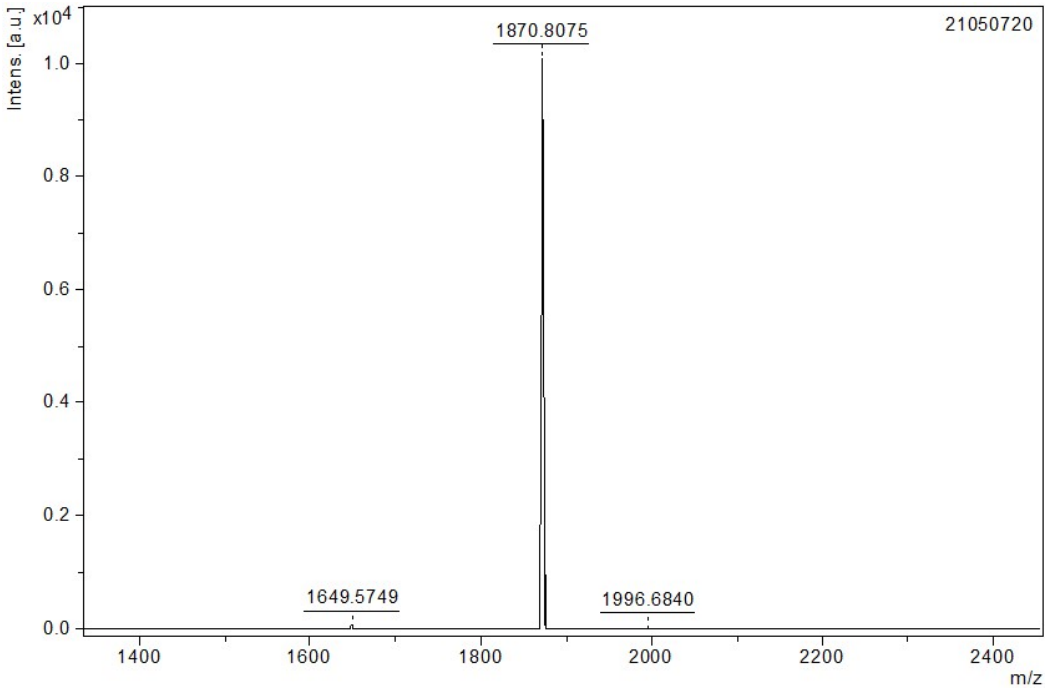


Figure S9. MALDI-TOF HRMS spectrum of **Flu(DPPdF)$_2$**. (calcd for $C_{113}H_{126}F_4N_4O_4S_6$：1870.8039)

3. TD-DFT calculated electronic transitions

Table S1. TD-DFT calculated electronic transitions of three compounds **Flu(DPP)$_2$**, **Flu(DPPsF)$_2$**, and **Flu(DPPdF)$_2$**.

Compound	State	E^{opt} (eV)	λ (nm)	f	Composition
Flu(DPP)$_2$	S1	1.87	662	3.6031	HOMO→LUMO (66%)
	S7	2.68	462	0.3396	HOMO→LUMO+2 (67%)
Flu(DPPsF)$_2$	S1	1.80	689	4.0517	HOMO→LUMO (65%)
	S18	3.27	379	0.3991	HOMO→LUMO+4 (57%)
Flu(DPPdF)$_2$	S1	1.79	692	3.9987	HOMO→LUMO (65%)
	S18	3.29	377	0.6001	HOMO-6→LUMO (46%)

4. CV curve of Fc/Fc+

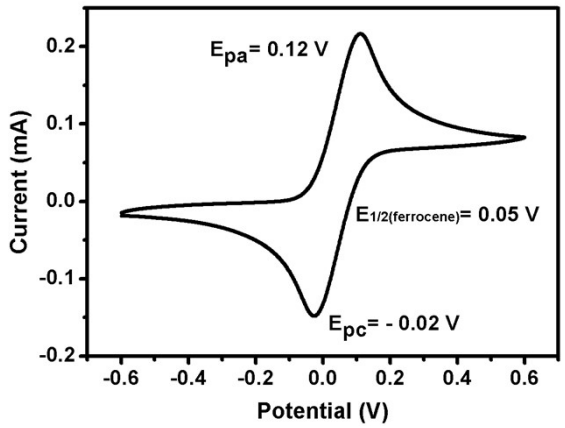


Fig. S10. The CV curve of **Fc/Fc**$^{+}$ in 0.1 M Bu_4NBF_4/CH_2Cl_2 solution at a scan rate of 100 mV s^{-1} under nitrogen.

5. Contact angle measurements

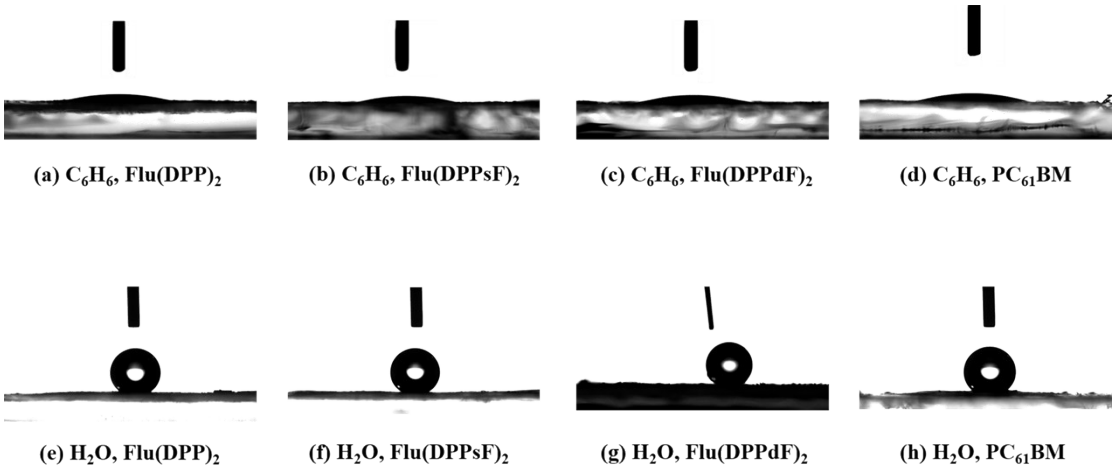


Fig. S11. Contact angle measurements of **Flu(DPP)$_2$**, **Flu(DPPsF)$_2$**, **Flu(DPPdF)$_2$** and $PC_{61}BM$

To investigate the miscibility and the interface properties of three SMDs and $PC_{61}BM$, contact angle measurements of the three SMDs and $PC_{61}BM$ were conducted. As we all know, ideal active layer morphology means good miscibility and similar contact angles of donors and acceptors.[7] As shown in **Fig. S11**, the contact angles are 13.5° and 140.3° for **Flu(DPP)$_2$** film in n-hexane and deionized water, 13.6° and 145.8° film for **Flu(DPPsF)$_2$** , 13.7° and 139.1° for **Flu(DPPdF)$_2$**, 16.0° and 136.8° for $PC_{61}BM$ film, respectively. Compare with **Flu(DPP)$_2$** and **Flu(DPPsF)$_2$**, the contact angle of **Flu(DPPdF)$_2$** is most similar to those of $PC_{61}BM$, indicating that there is most appropriate miscibility between **Flu(DPPdF)$_2$** and $PC_{61}BM$, which would be helpful for the formation of excellent bulk hetero-junction (BHJ)

morphology[7, 8].

6. References

1 A. B. Tamayo, B. Walker and T. Q. Nguyen, *J. Phys. Chem. C*, 2008, **112**, 11545–11551.

2 X. A. Jeanbourquin, A. Rahmanudin, X. Yu, M. Johnson, N. Guijarro, L. Yao and K. Sivula, *ACS Appl. Mater. Interfaces*, 2017, **9**, 27825–27831.

3 P. Sonar, G. M. Ng, T. T. Lin, A. Dodabalapur and Z. K. Chen, *J. Mater. Chem.*, 2010, **20**, 3626–3636.

4 F. Cheng, X. He, L. Yin, B. Xie and Y. Li, *Dye. Pigment.*, 2020, **176**, 108211.

5 H. Gao, Y. Li, L. Wang, C. Ji, Y. Wang, W. Tian, X. Yang and L. Yin, *Chem. Commun.*, 2014, **50**, 10251–10254.

6 J. Y. Pan, L. J. Zuo, X. L. Hu, W. F. Fu, M. R. Chen, L. Fu, X. Gu, H. Q. Shi, M. M. Shi, H. Y. Li and H. Z. Chen, *ACS Appl. Mater. Interfaces*, 2013, **5**, 972–980.

7 Y. Wang, S. Dong, Y. Miao, D. Li, W. Qin, H. Cao, L. Yang, L. Li and S. Yin, *IEEE J. Photovoltaics*, 2017, **7**, 550–557.

8 M. Li, S. Wang, C. Bao, Z. Liu, D. Bai, Z. Yang, W. Zhu, Q. Peng and Y. Liu, *J. Mater. Chem. C*, 2019, **7**, 12217–12230.