Supporting information

Synthesis of Asymmetric Imine Polymers for Highly Selective Sorting of Semiconducting Single-Walled Carbon Nanotubes by Two in One Strategy

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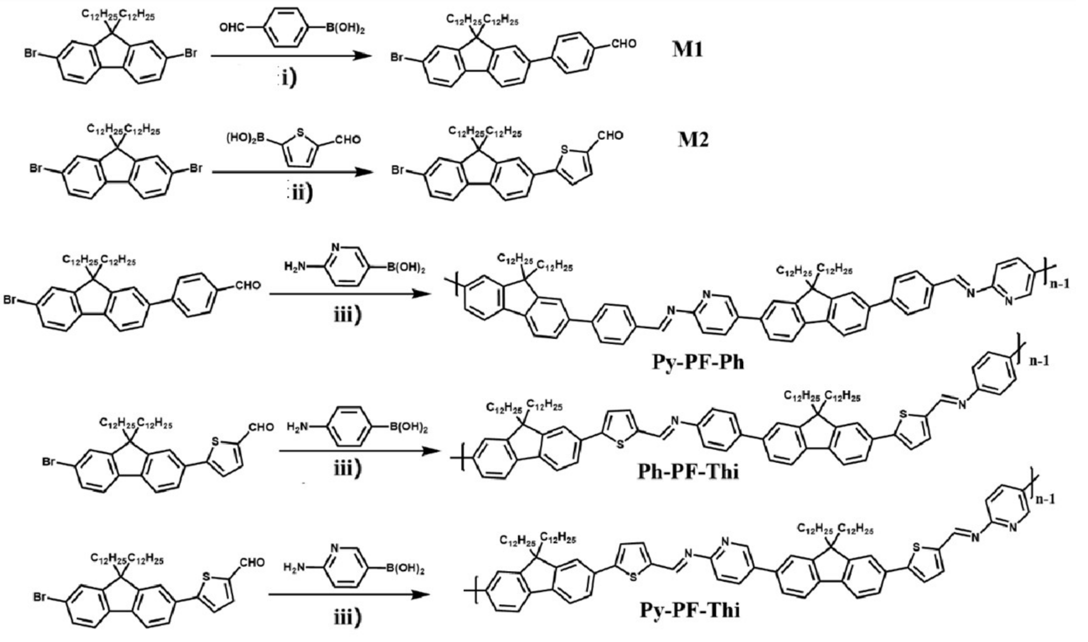
Polymer @SWCNTs dispersion preparation

In order to investigate the separation efficiency of synthesized polymers at various polymer/SWCNTs ratios, we should prepare the polymer@SWCNTs dispersion. The amounts of polymer ranging from 1 mg to 6 mg were dissolved in 6 mL of toluene, followed by complete dissolution through bath sonication. Then, 1 mg of SWCNTs was added, followed by sonication in a bath for 40 min at 480 W. Subsequently, the mixture was transferred to a 10 mL centrifuge tube and centrifuged at 15 °C for 30 minutes at a speed of 15300 rpm (19800g). After centrifugation, we collected 80% of the supernatant to obtain stable dispersion of polymer@SWCNTs for UV-Vis-NIR spectroscopy. To compare the selective separation ability of polymers for HiPCO-SWCNTs and Arc-SWCNTs, we prepared dispersions of PFO@SWCNTs and PCz@SWCNTs using commercially purchased polymers PFO and PCz, respectively, as well as a dispersion of SWCNTs in NMP for comparison.

Bare SWCNTs preparation

The polymer@s-SWCNTs dispersion was filtered through a nylon membrane with a 0.22 μm pore size. Subsequently, it is washed repeatedly with 10 mL of toluene and 10 mL of tetrahydrofuran (THF) solution, with black substance left on the filter membrane. The membrane with the black substance is then soaked in 2 mL of toluene solution and subjected to 10 minutes of ultrasonication. Afterward, the membrane is removed, and 0.3% trifluoroacetic acid (TFA) is added, followed by ultrasonication for another 10 minutes. The mixture is then centrifuged at 10000 rpm (9850g) for 10 minutes for collecting the precipitate. After washing repeatedly by toluene, the precipitate was then put in 2 mL of dichloromethane (DCM). The suspension of SWCNTs in DCM was then dropped onto a 1 cm×1 cm silicon wafer for Raman and XPS testing.



i) **$Pd(PPh_3)_4$, K_2CO_3, Toluene, H_2O, EtOH,105°C, underN_2, 36h**
ii) **$Pd(PPh_3)_4$, K_2CO_3, Toluene, H_2O, EtOH, 60°C, underN_2, 8h**
iii) **$Pd(PPh_3)_4$, K_2CO_3, Toluene, H_2O, EtOH, 105°C, underN_2, 36h**

Fig. S1 Chemical structure and synthetic route for M1, M2, P1, P2 and P3 in this work.

Table S1 Number-average molecular weight (Mn), weight-average molecular weight (Mw), polydispersity index (PDI), HOMO energy level (eV), LUMO energy level (eV), energy band gap (eV) and maximum absorption peak positions of polymers[c]

Polymer	Mn (KDa)[a]	Mw (KDa)[a]	PDI (Mw/Mn)[a]	HOMO (eV)[b]	LUMO (eV)[b]	Gap (eV)[b]	λ_{max} (nm)[c]
Py-PF-Ph (P1)	8.2	10.2	1.24	-5.45	-2.08	3.37	396
Ph-PF-Thi (P2)	8.6	15.2	1.77	-5.18	-2.15	3.03	427
Py-PF-Thi (P3)	3.2	11.3	3.54	-5.30	-2.31	2.99	438

[a] obtained by GPC;

[b] obtained by Gauss calculation;

[c] obtained by UV absorption spectrum.

Table S2 The s-SWCNTs sorted by our work and the reported polymers

Polymer	M11 valley [a]	Sonication（power and time）	Centrifugation（speed and time）	s-SWCNTs Purity [b]	Ref
P1	deeper	Bath sonication 40min	19800g 0.5 h	-	This work
Pcz	deeper	top-tip dispergator 45% amplitude 20 min 30% amplitude 15 min	60000g 2h	99.9%	Nano Research, **2021**, *14*, 4281.
Pcz	deeper	top-tip dispergator 30% amplitude 30min	20000g 1h	99.9%	Small, **2016,** *12*, 4993.
PF-PD	deeper	top-tip dispergator 50% amplitude 30min	22000g 0.5h	99.7%	Journal of the American Chemical Society, **2016**, *138*, 802.
Polymer1	deeper	top-tip dispergator	22000 g 0.5 h	-	Journal of the American Chemical Society, **2015**, *137*, 4328.
Polymer1	-	top-tip dispergator 30% amplitude	22000 g 45 min	99.7%	ACS Nano, **2017**, *11*, 5660.
PFODA	-	top-tip dispergator 50% amplitude 30min	22000 g 0.5 h	99.6%	Small, **2024**, 2403651.

[a] compared with commercial products from NanoIntegris (99.9%)

[b] measured from electrical device fabricated by the sorted s-SWCNTs

Table S3 Relationship between different chiral carbon nanotubes and chiral angle, diameter, excitation spectrum, emission spectrum

(n,m)	Chiral angle	Diameter(nm)	Emission wavelenghth	Excitation wavelength
(6,5)	26.996	0.757	983.935	569.171
(7,5)	24.504	0.829	1025.534	647.348
(7,6)	27.457	0.895	1126.805	650.870
(8,3)	15.295	0.782	952.058	661.976
(8,4)	19.107	0.840	1117.889	590.239
(8,6)	25.285	0.966	1174.465	721.185
(8,7)	27.796	1.032	1267.000	728.000
(9,2)	9.826	0.806	1126.195	547.894
(9,4)	17.480	0.916	1100.832	725.014
(9,5)	20.633	0.976	1251.021	674.765
(9,7)	25.872	1.103	1323.000	790.000
(9,8)	28.055	1.170	1399.852	826.305
(10,2)	8.948	0.884	1051.934	735.636
(10,5)	19.107	1.050	1249.174	793.195
(10,6)	21.787	1.111	1388.013	757.856
(11,1)	4.307	0.916	1251.534	607.382
(11,3)	11.742	1.014	1195.457	797.310
(12,4)	13.898	1.145	1340.252	863.132

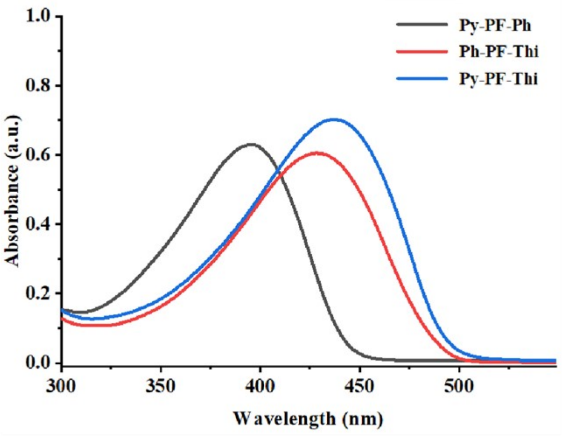


Fig. S2 UV absorption spectra of polymers Py-PF-Ph,Ph-PF-Thi and Py-PF-Thi in toluene.

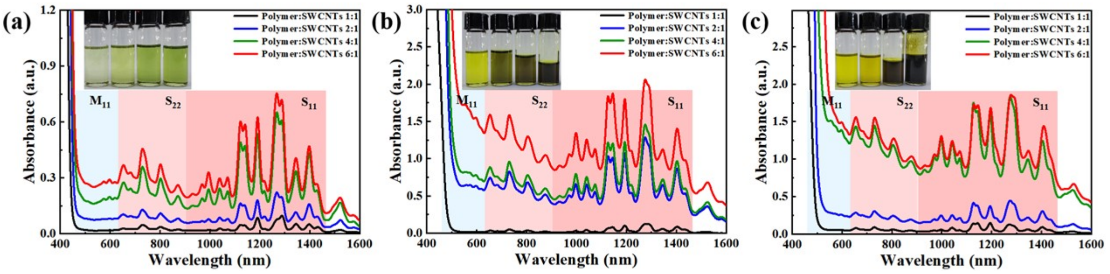


Fig. S3 UV-Vis-NIR absorption spectra of (a) Py-PF-Ph (P1), (b) Ph-PF-Thi (P2) and (c) Py-PF-Thi (P3) dispersed HiPCO-SWCNTs in different proportions and the carbon tube concentration is 0.16 mg/mL.

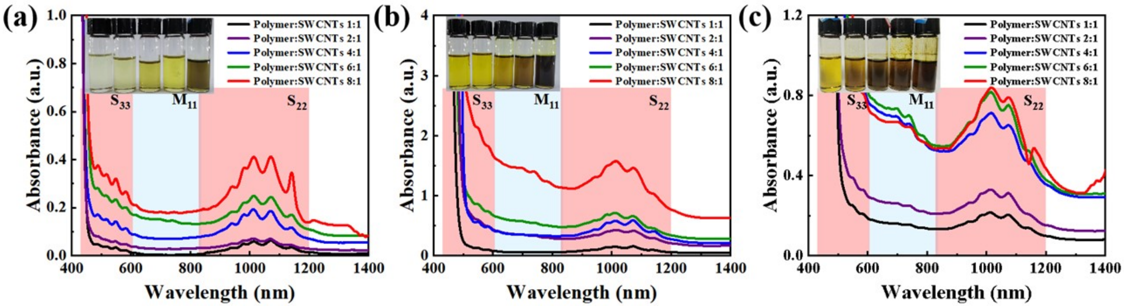


Fig. S4 UV-Vis-NIR absorption spectra of (a) Py-PF-Ph (P1), (b) Ph-PF-Thi (P2) and (c) Py-PF-Thi (P3) dispersed Arc-SWCNTs in different proportions and the carbon tube concentration is 0.16mg/mL.

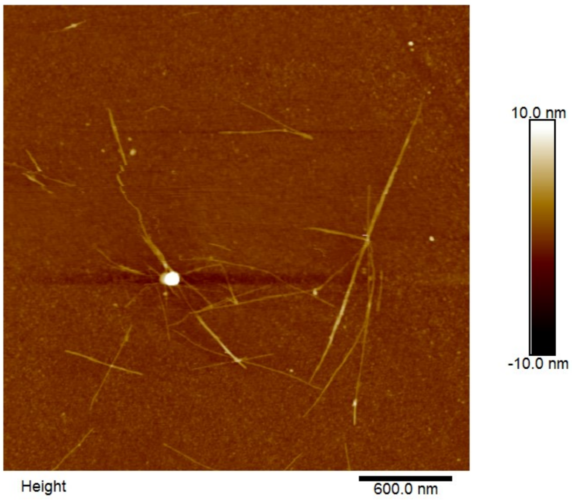


Fig. S5 AFM image of Py-PF-Ph (P1) dispersed s-SWCNTs on silicon wafer.

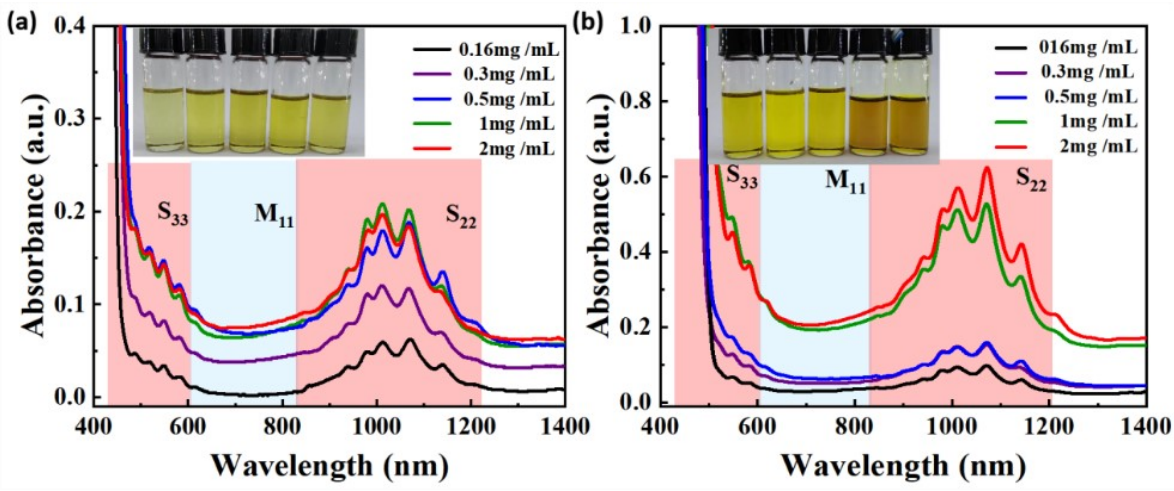


Fig. S6 UV-Vis-NIR absorption spectra of (a) Py-PF-Ph (P1) and (b) Ph-PF-Thi (P2) dispersed Arc-SWCNTs with different concentrations from 0.16 to 2 mg/mL. The ratio of polymer to Arc-SWCNTs is 1:1.

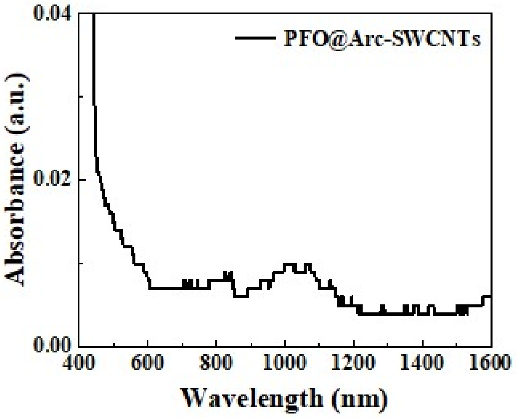


Fig. S7 UV-Vis-NIR absorption spectra of PFO (M_w: 5W) dispersed Arc-SWCNTs with concentration of 0.16 mg/mL. The ratio of polymer to Arc-SWCNTs is 1:1.

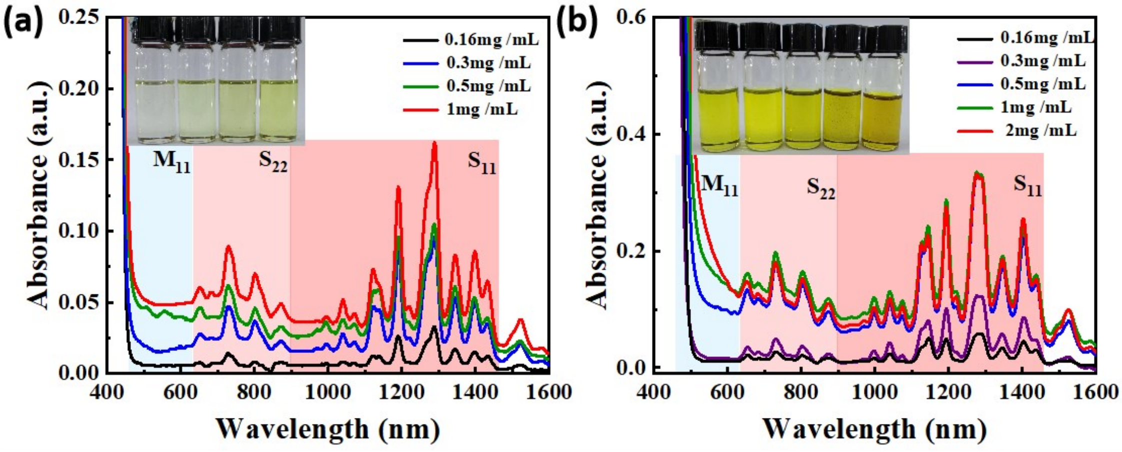


Fig. S8 UV-Vis-NIR absorption spectra of (a) Py-PF-Ph (P1) and (b) Ph-PF-Thi (P2) dispersed HiPCO-SWCNTs with different concentrations from 0.16 to 2 mg/mL. The ratio of polymer to HiPCO-SWCNTs is 1:1.

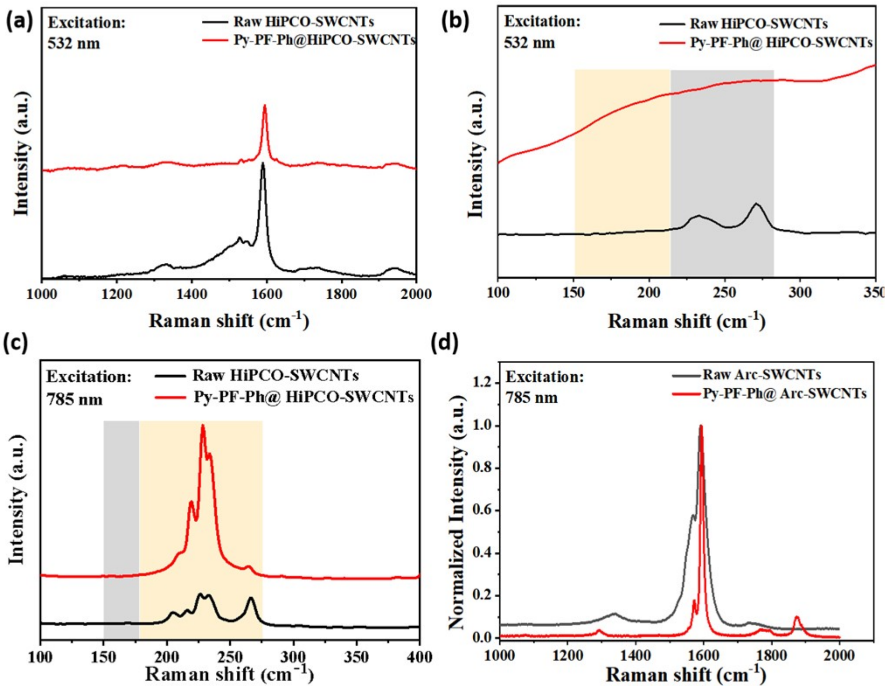


Fig. S9 (a) The G-band region of the Py-PF-Ph purified HiPCO-SWCNTs at an excitation wavelength of 532 nm. (b-c) The RBM region of Raman spectrum at laser wavelengths of 532 nm, and 785 nm, with the gray region representing the metallic type and the yellow region representing the semiconductor type SWCNTs. (d) The normalized G-band region of the Raman spectrum at the excitation wavelength of 785 nm.

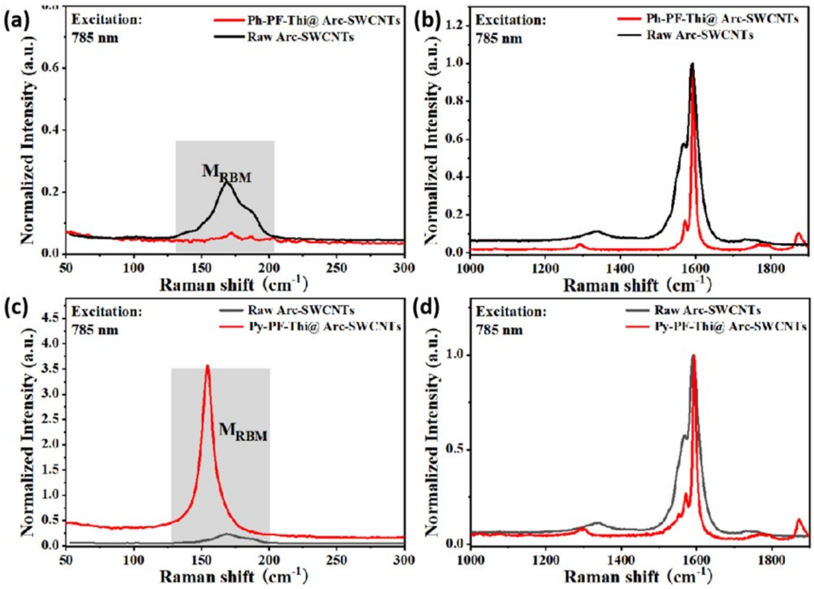


Fig. S10 (a) (c) RBM region of Raman spectrum for Ph-PF-Thi and Py-PF-Thi separated Arc-SWCNTs using 785 nm excitation wavelength. The gray area indicates the signal position of metallic SWCNTs. (b) (d) The normalized G-band region of the Raman spectrum for Ph-PF-Thi and Py-PF-Thi separated Arc-SWCNTs excited under laser wavelength of 785 nm.

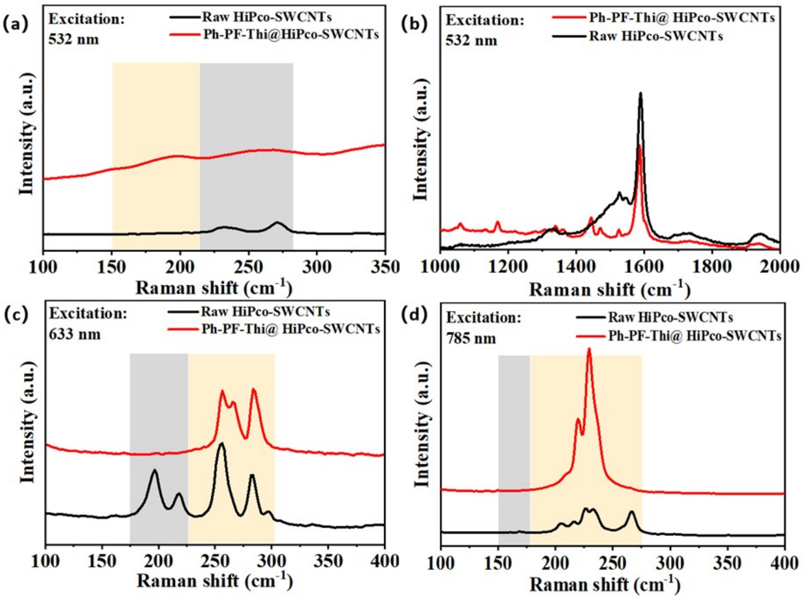


Fig. S11 The RBM region of Raman spectrum excited under laser wavelengths of (a) 532 nm (b) 633 nm and (c) 785 nm of the raw HiPCO-SWCNTs and Ph-PF-Thi purified HiPCO-SWCNTs. (b) the G-band region of Raman spectrum of the Ph-PF-Thi purified SWCNTs under the laser excitation wavelength of 532 nm. The gray region represents the metal type and the yellow region represents the semi conducting type SWCNTs, respectively.

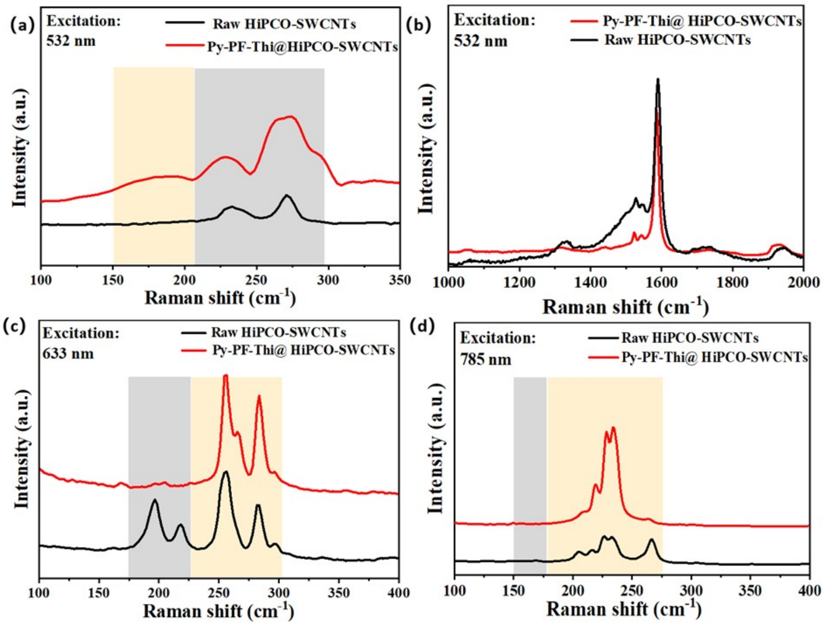


Fig. S12 The RBM region of Raman spectrum excited under laser wavelengths of (a) 532 nm (b) 633 nm and (c) 785 nm of the raw HiPCO-SWCNTs and Py-PF-Thi purified HiPCO-SWCNTs. (b) the G-band region of Raman spectrum of the Py-PF-Thi purified SWCNTs under the laser excitation wavelength of 532 nm. The gray region represents the metal type and the yellow region represents the semi conducting type SWCNTs, respectively.

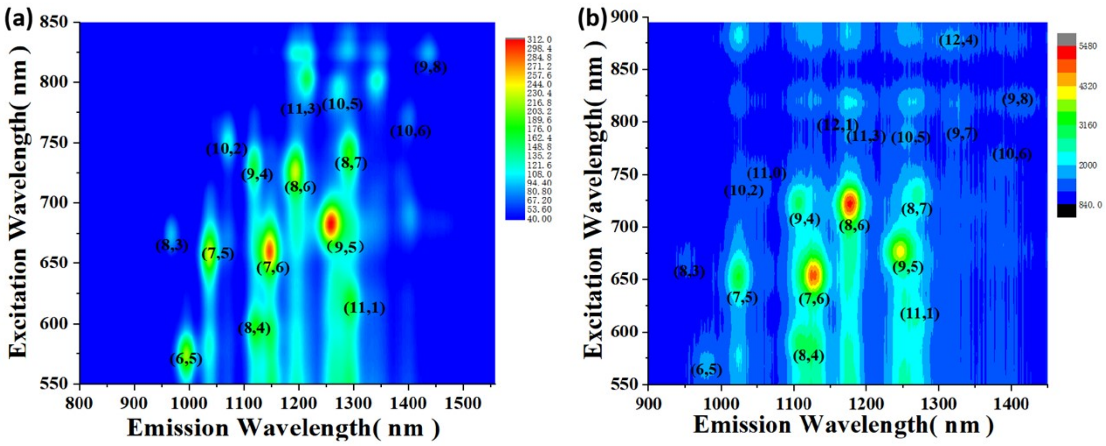


Fig. S13 The photoluminescence excitation spectra (PLE) of the polymers (a)Ph-PF-Thi (P2) and (b)Py-PF-Thi (P3) @HiPCO-SWCNTs 1:1 at a concentration of 0.17 mg/mL in toluene solution.

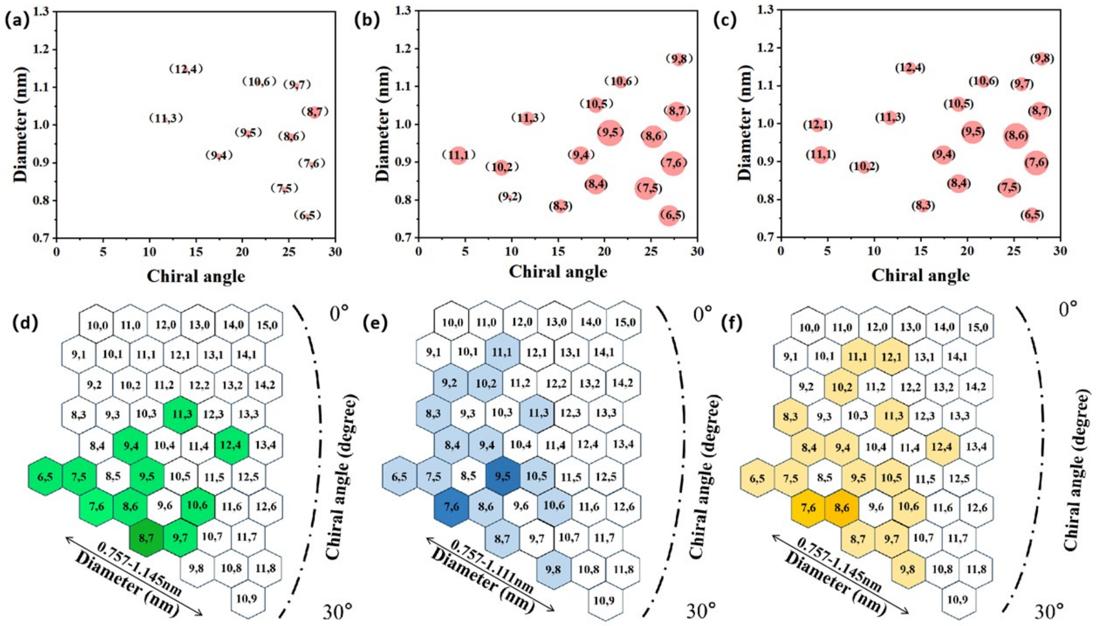


Fig. S14 The relationship between chiral angle and diameter, and the chiral diagram of P1, P2 and P3 @HiPCO-SWCNTs. The larger red circle in figure (a-c) and the darker hexagon color in figure (d-f) indicate that the luminous intensity of s-SWCNTs species is relatively strong which is proportional to the concentration.

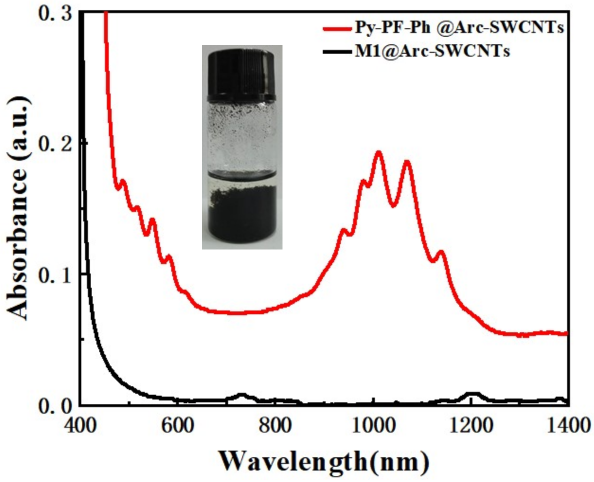


Fig. S15 Absorption spectra of M1@SWCNTs and P1@SWCNTs. The inset picture indicates the poor dispersion of M1 towards the raw SWCNTs.

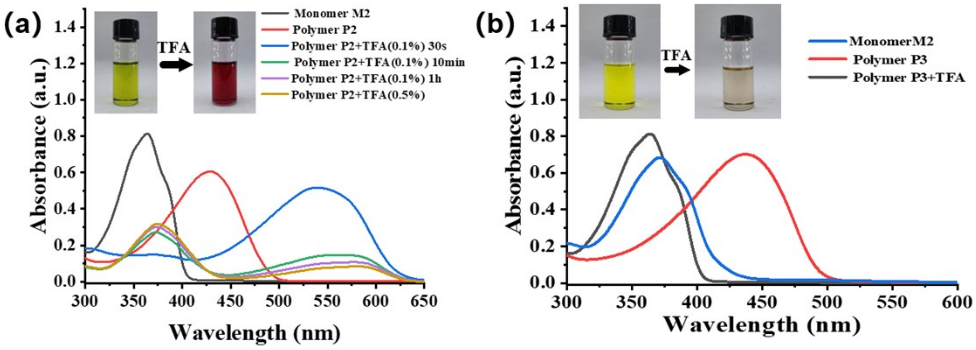
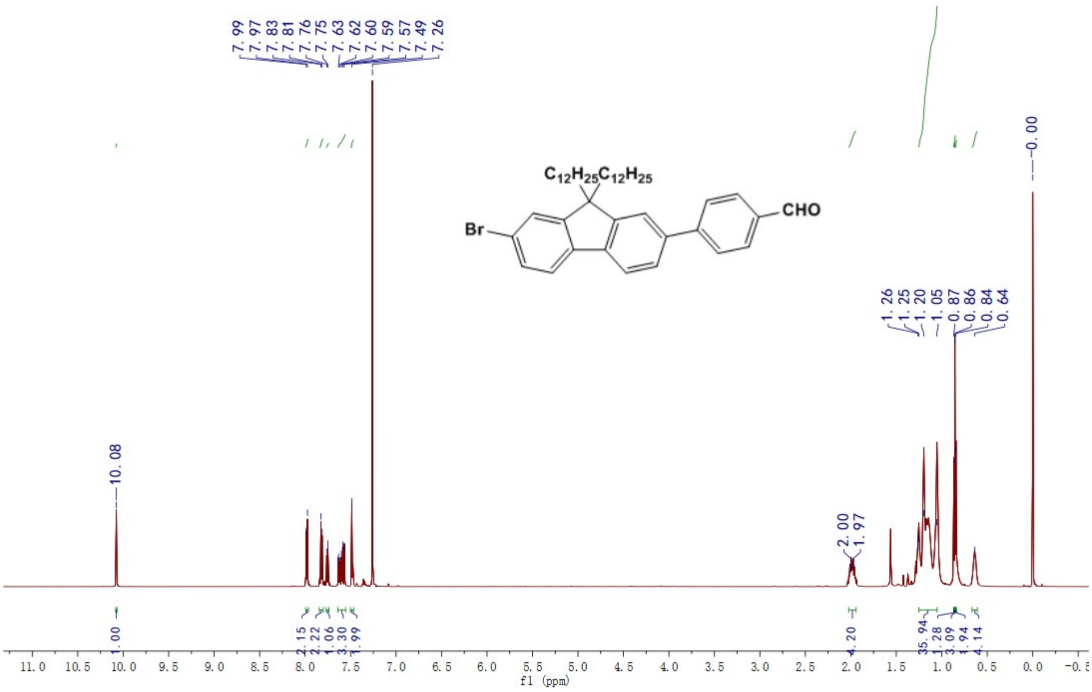
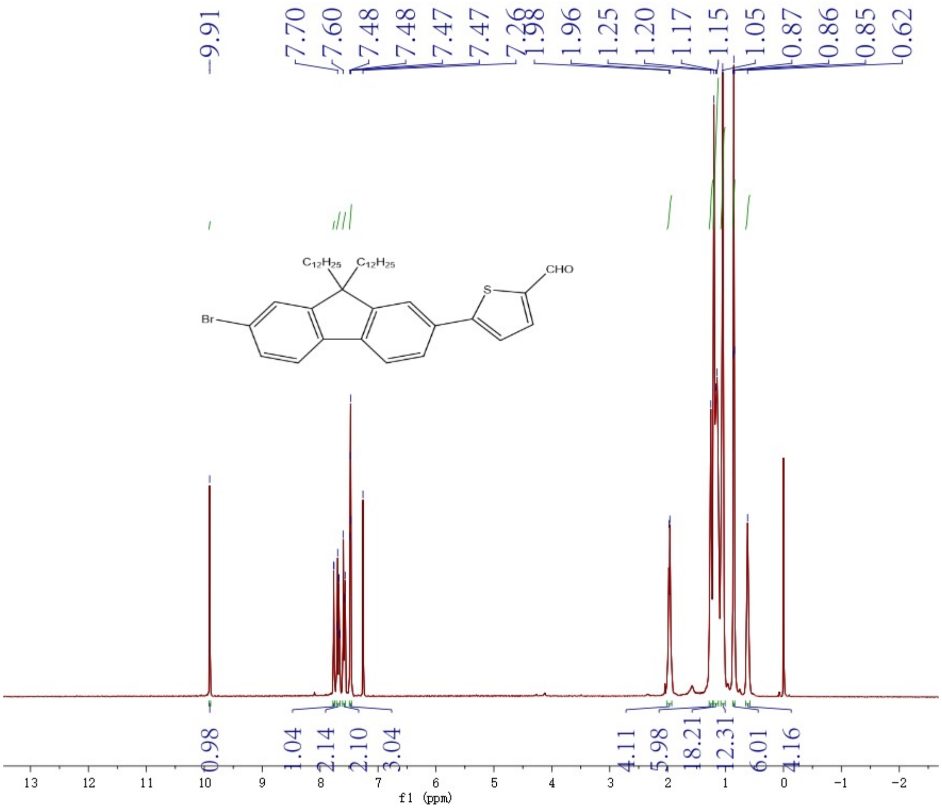


Fig. S16 Absorption spectra of polymers (a) P2 and (b) P3 before and after acid addition.

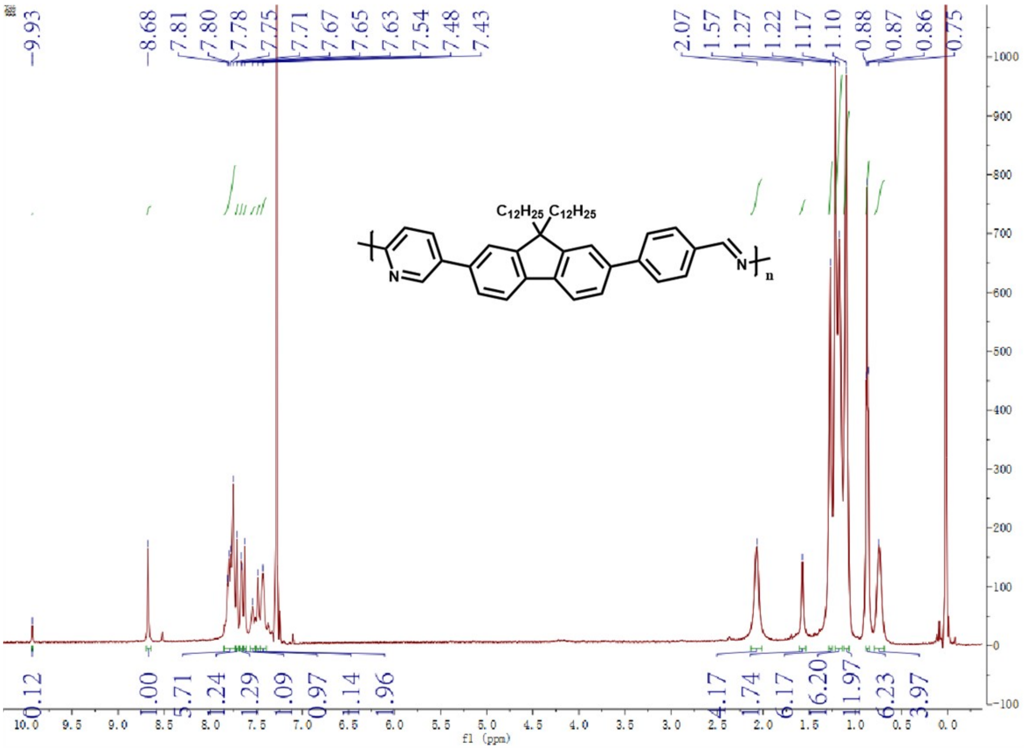
H^1 NMR spectra of all compounds in this paper.



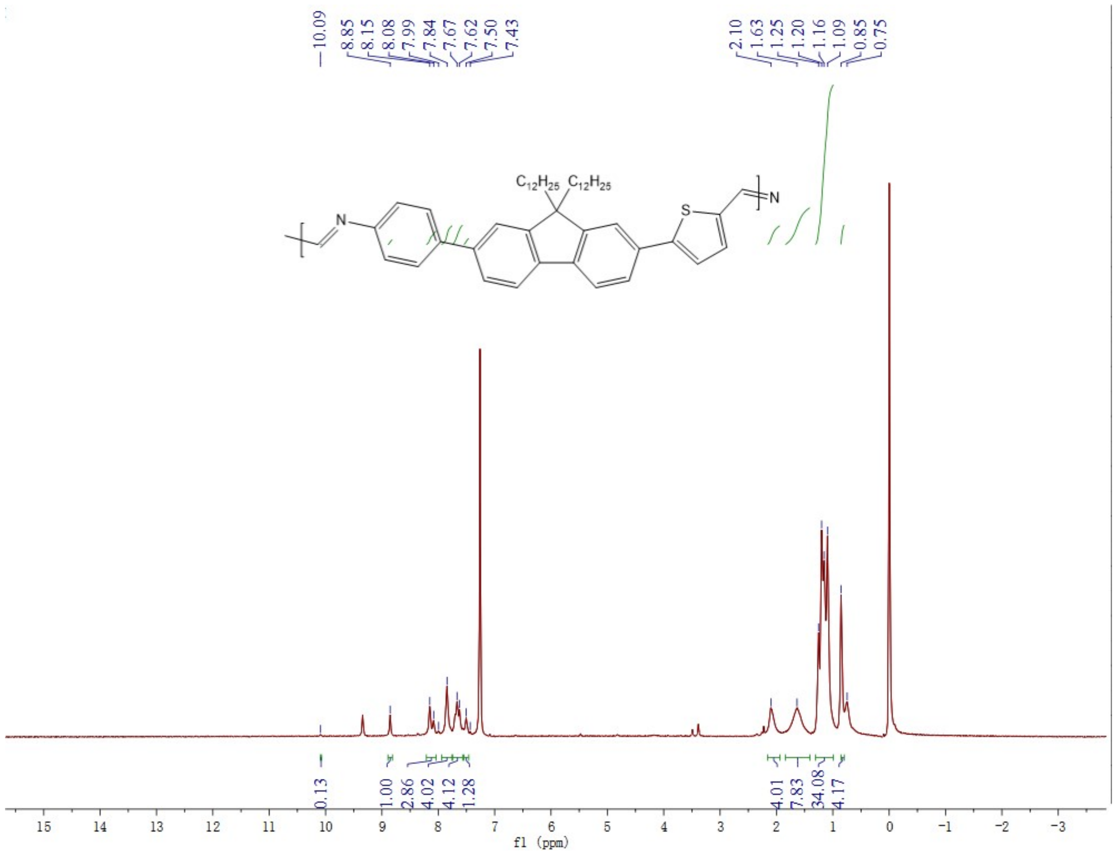
H^1NMR of M1



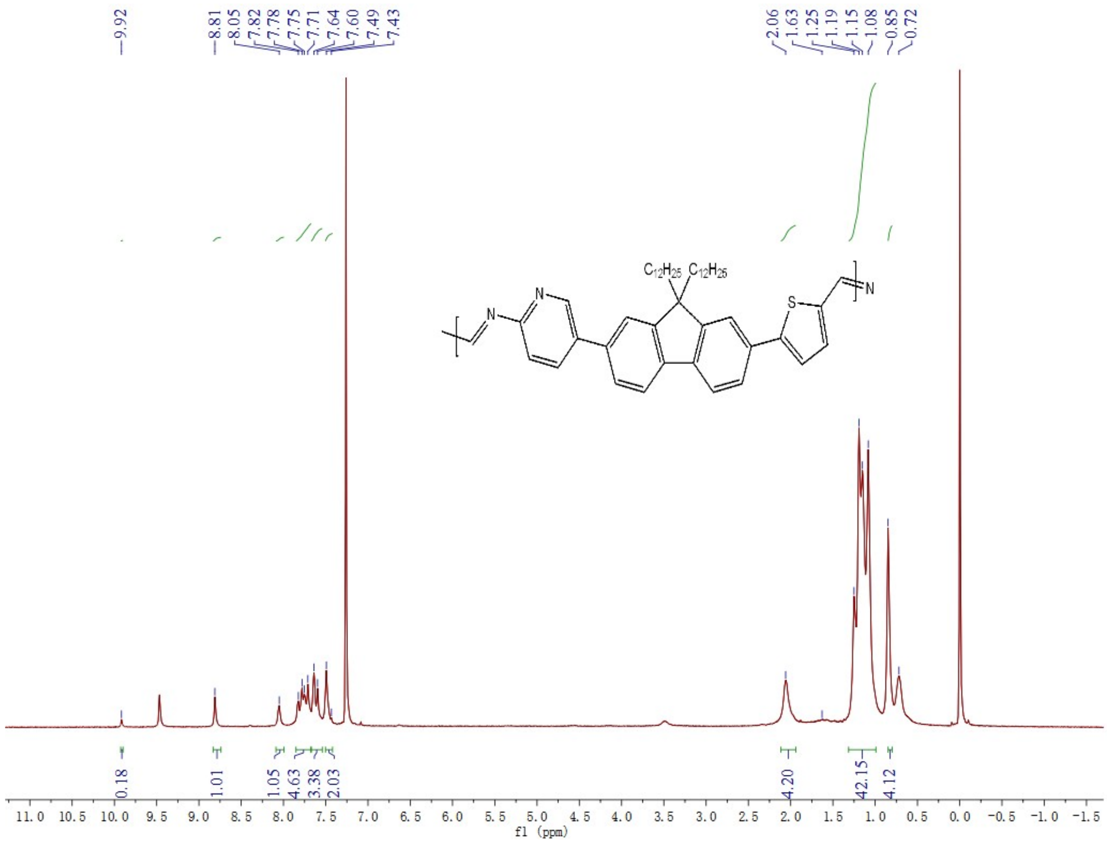
H^1NMR of M2



H^{1}NMR of P1



^{1}*H* NMR of P2


9.92
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7.75
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7.49
7.43
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1.19
1.15
1.08
0.85
0.72
C12H25 C12H25
N
N
S
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0.18
1.01
1.05
4.63
3.38
2.03
4.20
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4.12
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

H^{1}NMR of P3