Supplementary Information for

Enrichment of Highly Pure Large-Diameter Semiconducting SWCNTs by Polyfluorene Containing Pyrimidine Ring

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Characterization. Uv-vis-IR spectra were recorded by using a Shimadzu UV-3600 spectrophotometer (Kyoto, Japan) over a wavelength range from 250 to 1650 nm. Raman measurements were collected with a SENTERRA Raman spectrometer, equipped with a 20 mW argon ion laser (532 nm, grating 1200 lines / mm), a 100 mW Renishaw laser (785 nm, grating 1200 lines / mm). The lasers were set at less than 10% power. Photoluminescence excitation maps (PL) were acquired by FLS1000 Photoluminescence Spectrometer equipped with a 350 W Xe lamp and the NIR detector was cooling by liquid nitrogen. Slit width of both excitation and emission were 10 nm band-pass. PL maps were recorded with 5 nm intervals for both excitation (500 - 900 nm) and emission (900 - 1600 nm) wavelength.

Synthesis.[1-3] Poly(9,9-dioctylfluorene-alt-2-methyl pyrimidine) synthesis： 63.82 mg of 4,6-dichloro-2-methylpyrimidine, 251.59 mg of hydrazine monomer, 6.4 ml of THF, 6.4 ml of 3M K_3PO_4 (argon atmosphere for 20 minutes in advance) were added to the reaction flask, stirred well with continued argon gas protection. After 15 min, 28.6 mg of Pd(0) catalyst was added, and the mixture was stirred and heated at 75 ºC for 72 h. Argon gas protection during the reaction. After the end of the reaction, the copolymer was obtained in a yield of 60%.

Unsorted SWCNTs dispersion preparation: 350 mg SDBS dissolved in 35 ml deionized water, then added 5 mg plasma SWCNTs, ice bath 20 °C ± 5 °C, ultrasonic treatment for 2h, centrifugation at 20000rpm for 150min, supernatant was taken to measure the absorption curve.

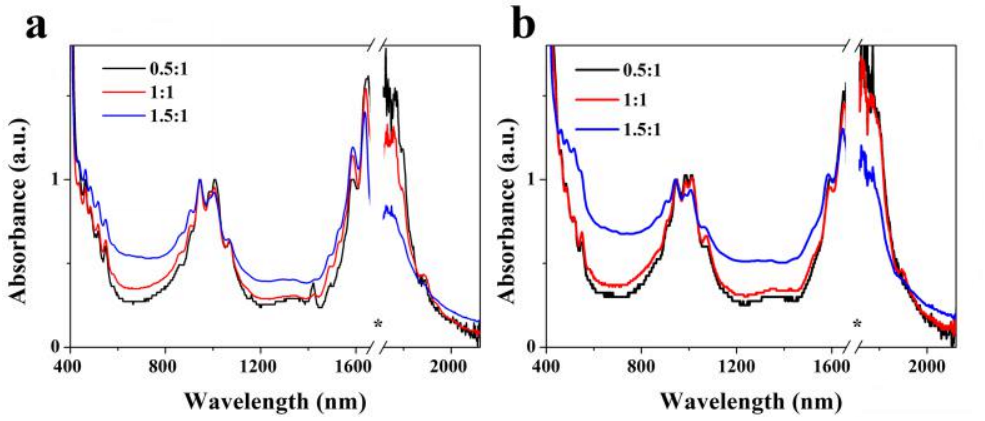


Fig. S1. The absorption of P1- and P2-enriched SWCNTs dispersion at different ratios in TL. The '*' is devoted by the absorbance of toluene solution, ranging from 1670-1710 nm.

Both for P1 and P2-enriched, the general trend can be seen from the Figure S1 that as the content of increasing polymer, less pure for the enrichment of sc-SWCNTs is obtained. And the Φ_i values of the two different ratios are calculated and shown in Figure S2. Wavenumber range is 8300 cm^{-1}-16000 cm^{-1}. Frankly, some other factors such as ultrasonic time and temperature, centrifugal speed et al. cannot be ignored. Under the condition of ensuring consistent and gentle conditions, the ratio of 0.5:1 for P1 was

selected as the object of further research.

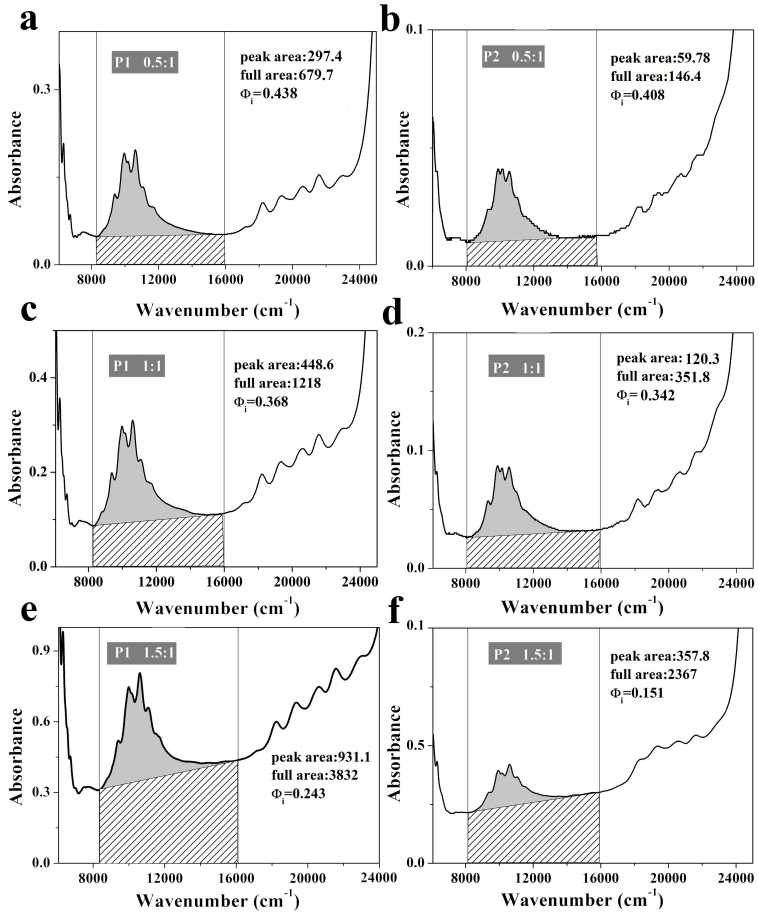


Fig. S2. The near-IR curve converted from absorption spectrum of P1- and P2-extracted SWCNTs dispersion.

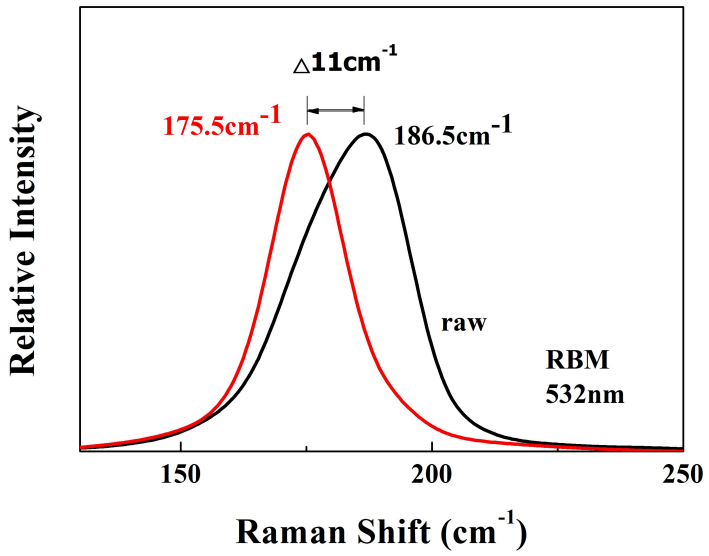
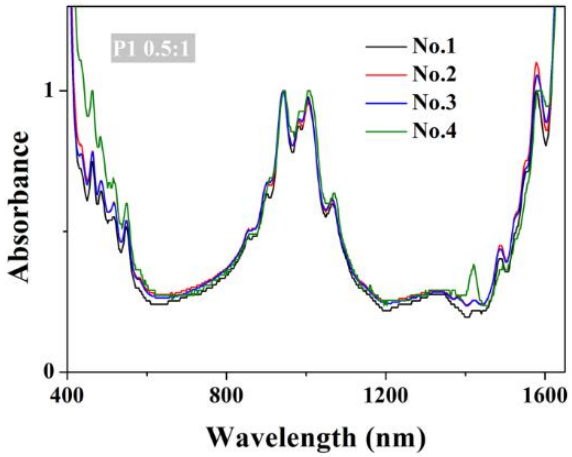


Fig. S3. The RBM range of Raman spectrum of P1-extracted at the ratio of 0.5:1 and raw SWCNTs, at 532 nm excitation wavelength.

According to the kataura plot and the formula ϖ_0=A/dt+B, it is clear that the diameter of SWCNT is negatively correlated with the Raman shift ϖ_0 corresponding to the RBM mode. What can be seen that the enriched sc-SWCNTs (red) exhibits red-shifted compared to the raw SWCNTs (black) with the difference of 11 cm^{-1}, and the peak width is relatively narrow, resulting the larger average diameter compared with raw SWCNTs, provides more possibilities for the application of pyrimidine-co-quinone polymer-enriched SWCNTs in the field of optoelectronic devices.



Sample	$Abs._{942nm}$	Φ_i^*
NO.1	0.087	0.465
NO.2	0.149	0.413
NO.3	0.197	0.438
NO.4	0.055	0.417

* The absorption spectrum is converted into near-IR analysis, and the Φ value is the ratio of the peak area of the envelopes of S22 and M11, and the interval is 8300 cm^{-1}-16000 cm^{-1}.

Fig. S4. Absorption spectra of four parallel experiments of P1 enriched SWCNTs at the ratio of 0.5:1.

The figure S4 shows the absorption curve of the normalized at 942 nm sample of four parallel samples of P1/SWCNTs at the ratio of 0.5:1, for confirming the repeatability of the polymer extraction. The absorption intensity (Φ_i value) corresponding to the 942 nm peak are 0.197 (0.438), 0.149 (0.413), 0.087 (0.465), 0.055 (0.417) respectively.

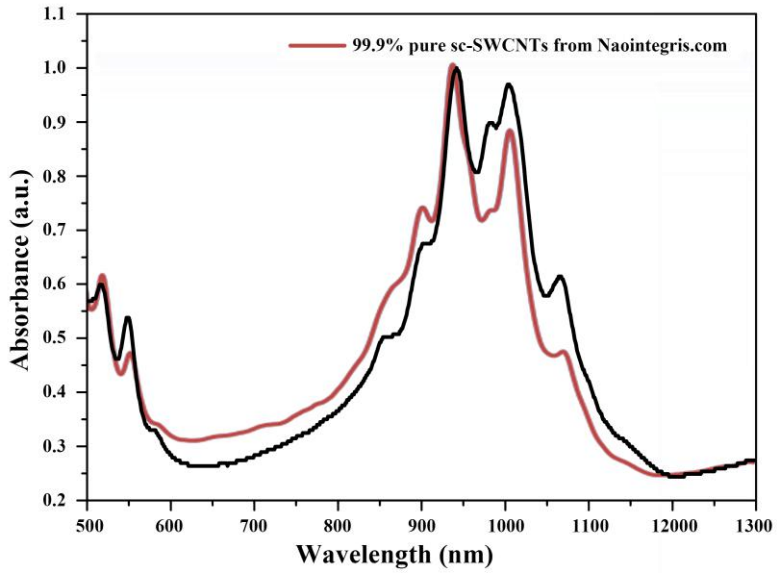


Fig. S5. The absorption spectra of P1-enriched high-purity sc-SWCNTs were compared with the sc-SWCNTs with high purity of 99.9% from nanointegris.

It can be seen from Figure S5 that by comparing the absorption spectra of our P1-enriched sc-SWCNTs with spectrum of high purity of 99.9% from nanointegris company, the purity of the P1-enriched product (NO.3 sample, Φ_i=0.417) is very high, greater than 99.9%.

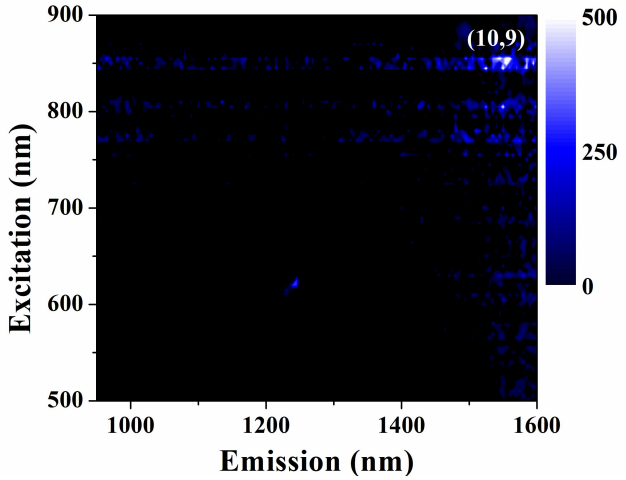


Fig. S6. Photoluminescence spectra of P1/SWCNTs in TL at ratio of 0.5:1.

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