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Supporting Information

Sorting and Decoration of Semiconducting Single-walled Carbon Nanotubes via Quaternization Reaction

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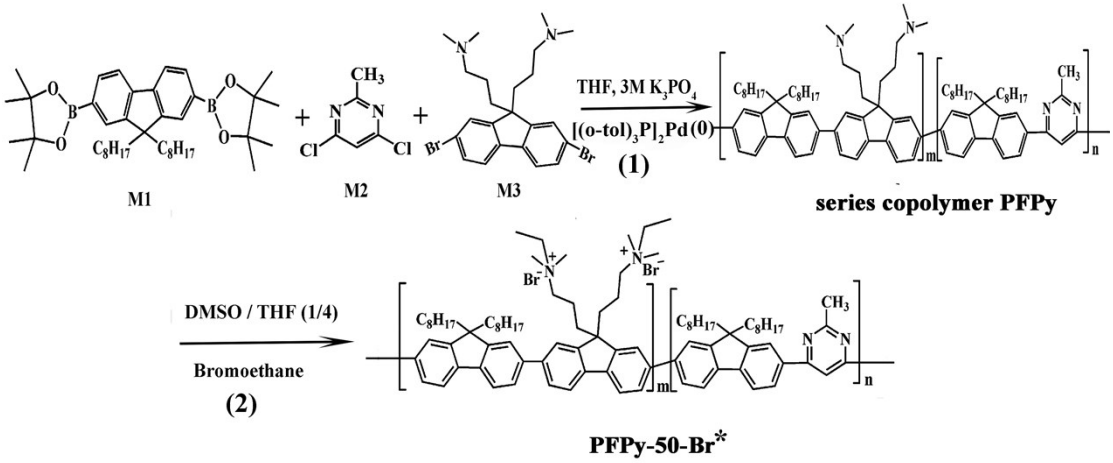
1. Materials and Characterization

All the chemicals used were of analytical grade. Dichloromethane (CH_2Cl_2), toluene (TL), [(o-tol)$_3$P]$_2$Pd (0) and methanol (MeOH) were purchased from Shanghai Fine Chemical Materials Research Institute., Shanghai, China. Reflux under 110℃, toluene was distilled off in the metal sodium powder and dried.

PAFPD-50-Br*: Poly (9, 9-bis (3′- ((N, N- dimethyl)- N- ethylammonium) -propyl) -2, 7- fluorene)- alt- 2, 7- (9, 9- dioctylfluorene) dibromide (PFPy-50-Br*) was synthesized according to the literature [1]. The neutral polymer PFPy-50 (50 mg) was carried out under the protection of argon by stirring with bromoethane in DMSO/THF (1/4) at 70℃ for 5 days. The synthetic process of polymers were shown in Scheme S1.



Scheme S1. The synthetic route of copolymers.

2. Enrichment of sc-SWCNTs with a series of polymers

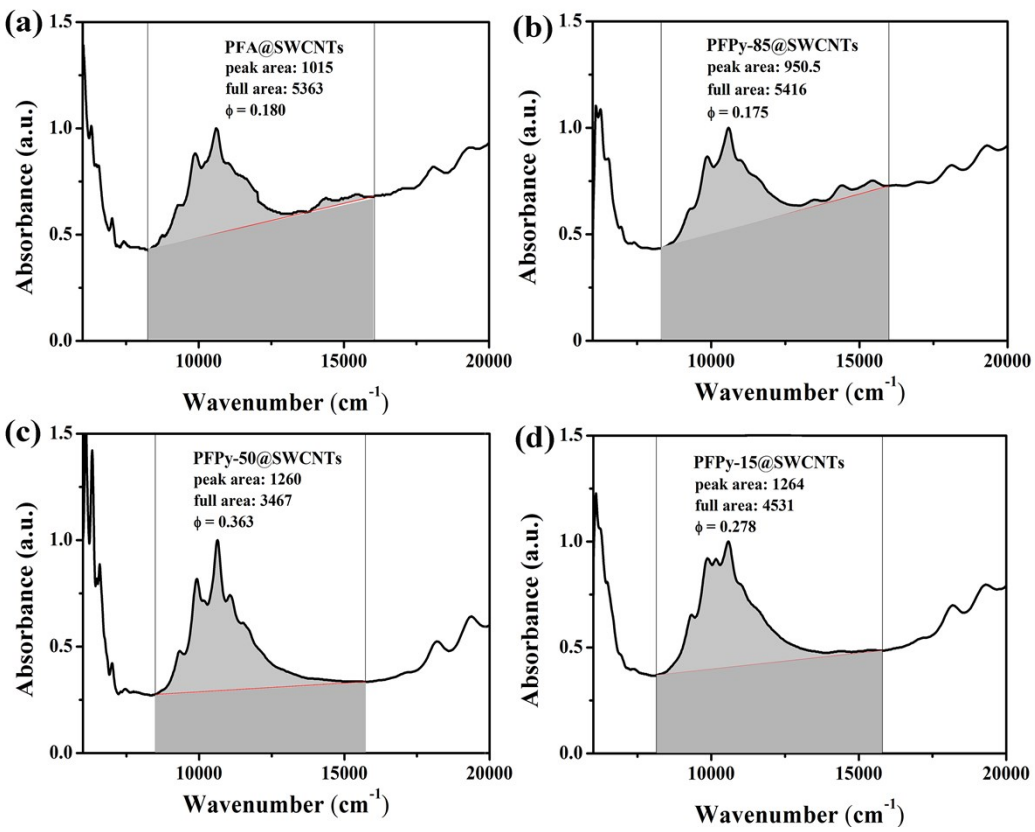


Figure S1. ϕ value evaluation of sc-SWCNTs separated by (a) PFA, (b) PFPy-85, (c) PFPy-50 and (d) PFPy-15, converted from absorption spectra, ranging from 8400 cm^{-1} to 16000 cm^{-1}.

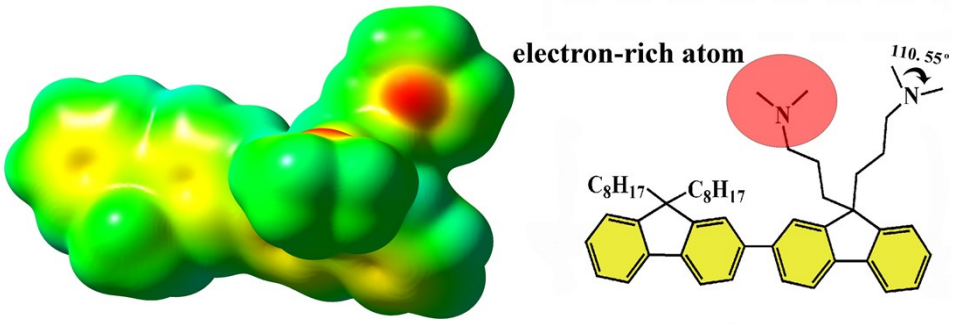


Figure S2. The electron-density maps of PFA. Red denotes electron-rich regions, green denotes less electron-rich regions and blue denotes electron-poor regions.

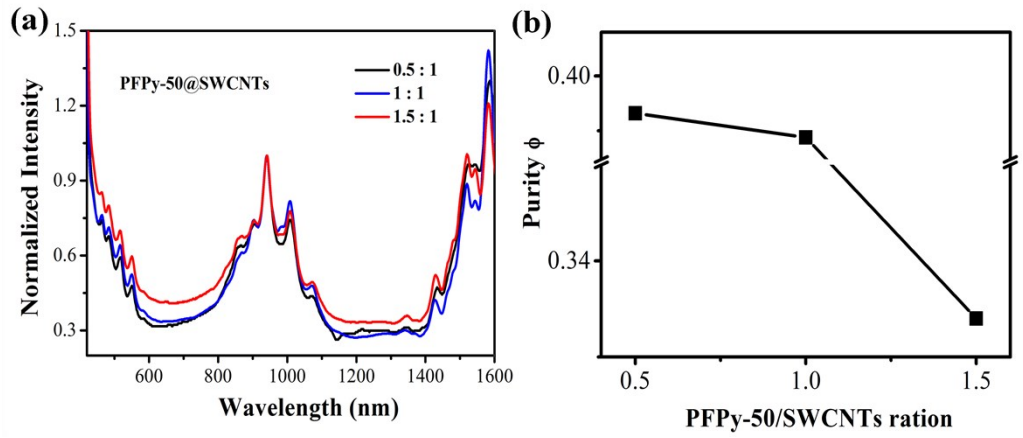


Figure S3. (a) UV-Vis-NIR spectra of PFPy-50: raw SWCNTs at 0.5:1, 1:1, and 1.5:1; (b) ϕ value of sc-SWCNTs purity separated PFPy-50 with different proportions.

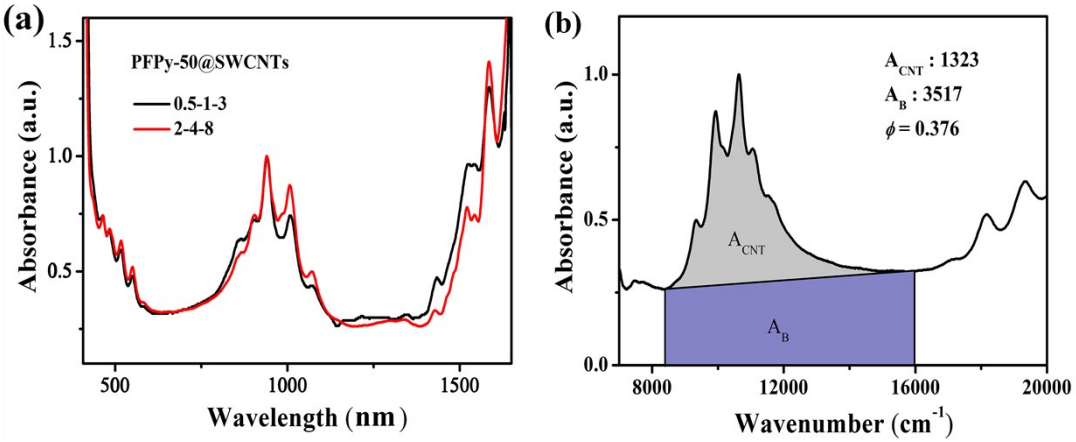


Figure S4. (a) Comparison of absorption spectra dispersion obtained from PFPy-50: raw SWCNTs at 0.5: 1 (black line) and 2: 4 (red line), respectively. (b) ϕ value evaluation of PFPy-50@SWCNTs dispersion with PFPy-50: raw SWCNTs at 2:4.

Different mass ratios operations of the polymer and raw SWCNTs: The different mass (0.5, 1.0 and 1.5 mg) of the PFPy-50 were dissolved in 3.0 ml of TL and filtered through 0.22 μm pore size filters before 1.0 mg of raw single-walled carbon nanotubes (raw SWCNTs) were added. The PFPy-50@SWCNTs dispersion was obtained by use of 200 W ultrasonication for 2 h under ice water (20℃±5℃). The dispersion was centrifuged at 20,000 rpm and 10℃ to obtain a supernatant, which was used as a PFPy-50@SWCNTs dispersion.

3. The process of quaternization PFPy-50@SWCNTs complex

The PFPy-50/SWCNTs (0.5/1) ratio of excellent sorting purity were selected, and the mixed ratio was enlarged four times to 2/4 putting in 8 ml of TL. Then the mixture was sonicated for 2 h in an ice bath with temperature control. And PFPy-50@SWCNTs dispersion (Figure S5①) obtained to centrifuged 20,000 rpm for 30 min at 10℃, which the sc-SWCNTs purity reached ϕ=0.376 (**Figure S4b**). Two groups of PFPy-50@SWCNTs dispersion were prepared under the same conditions as above. One group of TL with the PFPy-50@SWCNTs dispersion evaporated, and the residues of the complex was dissolved in 4 mL of MeOH to sonicate 20 min for UV-vis-INR detection (as a **sample before QR in MeOH**). The other group of TL evaporated, and the residues of the complex were dissolved in 5 ml of THF. Then 0.6 ml of DMSO and 70 uL of bromoethane were added under the protection of argon. After 5 days of reaction (Figure S5②), it was recrystallized from ethyl acetate and filtered through a 0.22 um nylon 66 filter (Figure S5③). Finally, the recrystallized PFPy-50-Br@SWCNTs complex was dispersed in 4 mL of MeOH by sonication for 20 min, as a **sample after QR in MeOH** (Figure S5④).

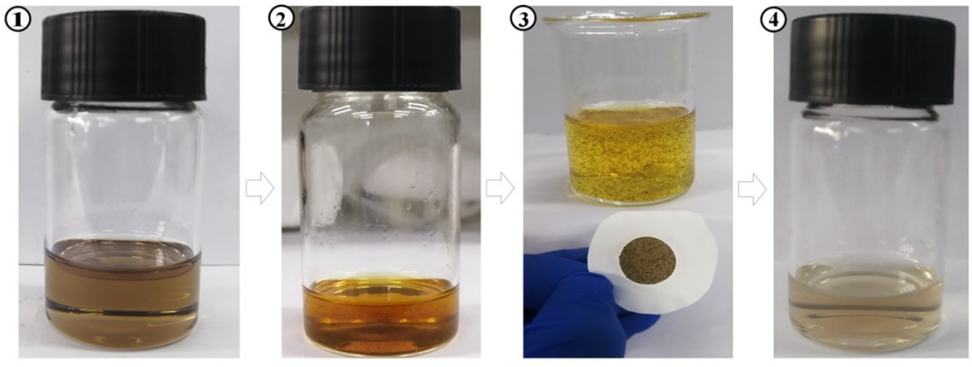


Figure S5. The whole process of the quaternization reaction for PFPy-50@SWCNTs was functionalized into alcohol-soluble PFPy-50-Br@SWCNTs.

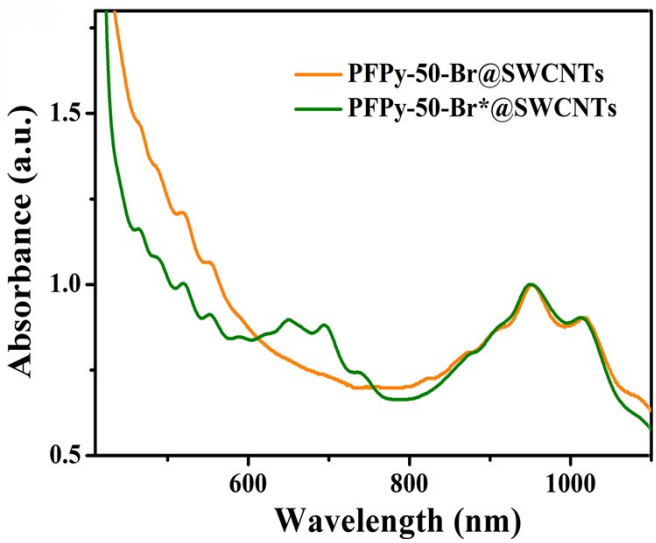


Figure S6. UV-vis-NIR spectra with PFPy-50-Br@SWCNTs (orange line) of post-QR and PFPy-50-Br*@SWCNTs dispersion in MeOH (green line).

References

1. Maimaiti, Y.; Maimaitiyiming, X. Fluorescence quenching of methanol-soluble polypyrimidine by aluminum ion. Materials Express. 2020, 7, 1177-1188.