

**Supporting Information**

**Polymer Removal and Dispersion Exchange of (10,5) Chiral Carbon Nanotube with Enhanced 1.5  $\mu\text{m}$  Photoluminescence**

Yahui Li,<sup>ab</sup> Ye Liu<sup>b</sup>, Feng Jin<sup>b</sup>, Leitao Cao<sup>b</sup>, Hehua Jin<sup>ab</sup>, Song Qiu<sup>\*ab</sup> and Qingwen Li<sup>\*ab</sup>

<sup>a</sup> School of Nano-Tech and Nano-Bionics, University of Science and Technology of China, 96 Jinzhai Road, Hefei 230026, China

<sup>b</sup> Division of Advanced Nano-Materials, Suzhou Institute of Nanotech and Nano-bionics, Chinese Academy of Science, 398 Ruoshui Road, Suzhou 215123, China

\*Corresponding author: [sqiu2010@sinano.ac.cn](mailto:sqiu2010@sinano.ac.cn); [qwli2007@sinano.ac.cn](mailto:qwli2007@sinano.ac.cn)

## Experimental Section

### Materials

Raw HiPCO SWCNTs were purchased from Nanointegris Inc. and utilized without modification. The chemical reagents used in the experiment, such as toluene, tetrahydrofuran, and trichloromethane, were procured from China National Pharmaceutical Group Chemical Reagent Co., Ltd., with a purity of analytical grade. Trifluoroacetic acid (TFA), sodium dodecyl sulfate (SDS), and 4-Methoxybenzenediazonium tetrafluoroborate were purchased from Shanghai Aladdin Biochemical Technology Co., Ltd. The polymers poly[(9,9-dioctylfluorenyl-2,7-diyl)-alt-(1,4-benzo-{2,1'-3}-thiadiazole)] (F8BT) and 9-(1-octylonoyl)-9H-carbazole-2,7-diyl (PCZ) were synthesized through Suzuki polymerization reactions, as detailed in previous literature<sup>1,2</sup>.

### Characterization Tools

Absorption spectra were collected on a UV-vis-NIR spectrophotometer (Cary 5000, Agilent) with an optical path of 10 mm. A double beam mode was used with a pure solvent quartz cuvette placed in the reference channel. NIR-fluorescence spectroscopy was performed on a Fluorlog spectrofluorometer equipped with a 450 W xenon lamp and a liquid nitrogen-cooled InGaAs line camera from Horiba Inc.

### Preparation of SWCNTs Dispersions in Organic Phase

Preparation of semiconducting SWCNTs: Dispersants PCZ (5 mg) and SWCNTs (5 mg) were mixed in toluene (10 mL). The solutions were ultrasonicated with a top-tip dispersator (Sonics VC500) for 1 h at an amplitude level of 30%, and then were centrifuged at 20 000 g for 1 h (Allegra X-22R centrifuge) to remove the bundles and insoluble materials. The supernatants were collected for follow-up experiment.

Preparation of (10,5) SWCNTs: Dispersants F8BT (5 mg) and SWCNTs (10 mg) were mixed in toluene (10 mL). The solutions were ultrasonicated with a top-tip dispersator (Sonics VC500) for 1 h at an amplitude level of 30%, and then were centrifuged at 10 000 g for 1 h (Allegra X-22R centrifuge) to remove the bundles and insoluble materials. The supernatants were collected for follow-up experiment.

### System Transposition of SWCNTs

The solution inversion of HiPCO semiconducting SWCNTs and (10,5) SWCNTs in organic phase can be achieved using a general transposition strategy. Firstly, the initial organic phase dispersion is vacuum-filtered, and the filtrate can be recycled for the selective separation of SWCNTs. The obtained SWCNTs filter cake is redispersed in toluene solvent, effectively removing the majority of free polymers from the solution, leaving only polymers coating the surface of SWCNTs. Subsequently, 1% volume ratio trifluoroacetic acid (TFA) is added to the solution, inducing the coagulation of SWCNTs. The resulting precipitate is collected through centrifugation at 2000 g. The precipitate is then redispersed in toluene under 2-4 minutes of tip ultrasound or 5-8 minutes of water bath ultrasound, and the addition of TFA is repeated multiple times until the SWCNTs can no longer be redispersed in toluene. Chloroform is then introduced for further SWCNT redispersion. Following this, TFA is added again, leading to SWCNT agglomerations, and the precipitate is collected through centrifugation at 2000 g. Finally, the precipitate is introduced into a 1% volume ratio sodium dodecyl sulfate (SDS) solution, subjected to 1-hour sonication, and then being centrifuged to remove the non-dispersible SWCNTs. The advantage of our method is that SWCNTs do not undergo strong annealing, repeated filtering, and strong centrifugation processes, so they can maintain a relatively loose state and are not easy to form tight tube bundles, making it easy for SWCNTs to be redispersed

in new solvents. The mild ultrasound (within 10 minutes) used in this method minimize the introduction of additional defects.

### Introduction of $sp^3$ defects of SWCNTs

For HiPCO semiconducting SWCNTs, initially prepare a dispersion of SWCNTs with an absorbance at the  $S_{11}$  region of approximately 1200 nm, achieving an absorbance of around 0.2. For the 4-Methoxybenzenediazonium tetrafluoroborate, prepare a solution with a concentration of  $0.02 \text{ mg}\cdot\text{ml}^{-1}$  in  $50 \mu\text{l}$ , diluted in 5 ml of an aqueous dispersion. Shield the reaction from light by covering the glass bottle with tin foil and let it react for 24 hours. After the reaction, filter the solution to form the filter cake and wash the filter cake successively with tetrahydrofuran and deionized water. Finally, redisperse it in 5 ml of a 1% SDS solution and await subsequent characterization.

For (10,5) SWCNTs, begin by preparing a dispersion of SWCNTs with an absorbance at the  $S_{11}$  region of approximately 1275 nm, achieving an absorbance of around 0.3. Simultaneously, for the 4-Methoxybenzenediazonium tetrafluoroborate, prepare a solution with a concentration of  $0.01 \text{ mg}\cdot\text{ml}^{-1}$  in  $30 \mu\text{l}$ , diluted in 5 ml of an aqueous dispersion. Shield the reaction from light by covering the glass bottle with tin foil and let it react for 24 hours. After the reaction, vacuum filter the solution to form a filter cake and wash the cake successively with tetrahydrofuran and deionized water. Finally, redisperse it in 5 ml of a 1% SDS solution and await subsequent characterization.

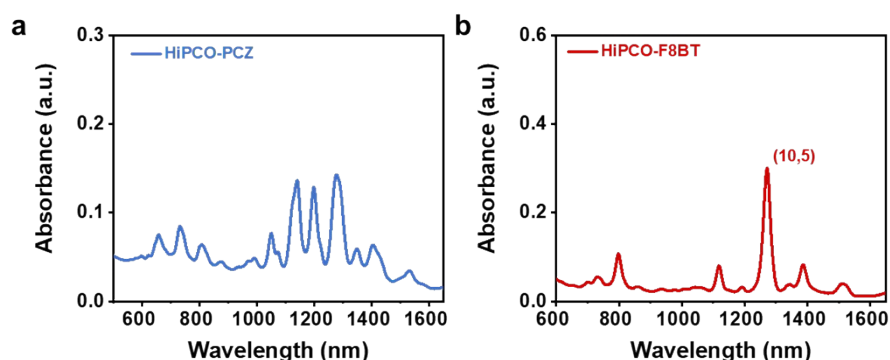


Figure. S1 Absorbance spectra of HiPCO SWCNTs separation using (a) PCZ and (b) F8BT

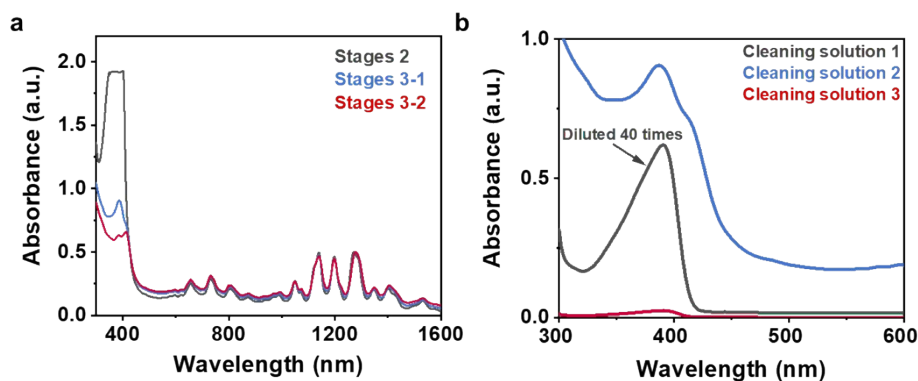
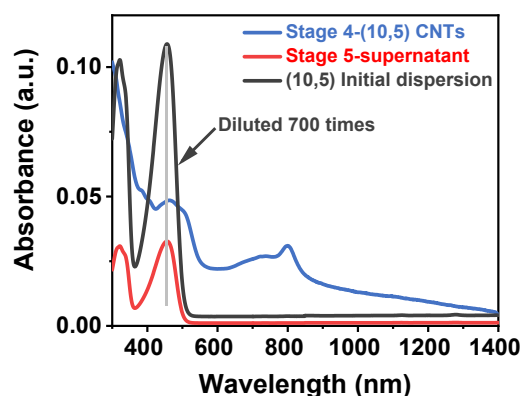
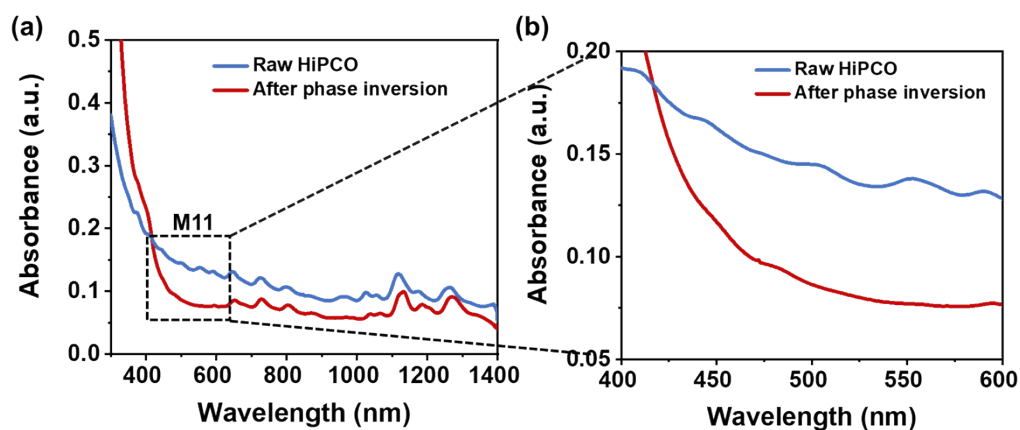


Figure. S2 (a) The absorption spectra of HiPCO s-SWCNTs after redispersion in toluene solvent after one THF rinsing and two TFA rinsing. (b) The absorption spectra of the filtrate and the supernatant after three cleaning cycles. In (a) and (b), the legend texts share colors with their corresponding plots.

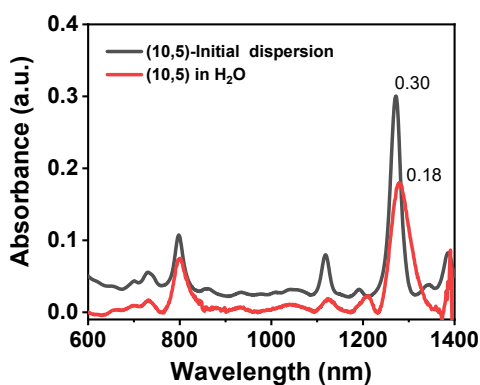


**Figure. S3.** The absorption spectra of polymers at different stages. We use the absorption peak at 455 nm to represent the F8BT polymer content.

The ratio between the remaining polymers and the total polymers is estimated by analyzing polymer peak intensity in absorption spectra. The remaining ratio of polymers is  $<0.1\%$ , and therefore the removal ratio is  $>99.9\%$ .

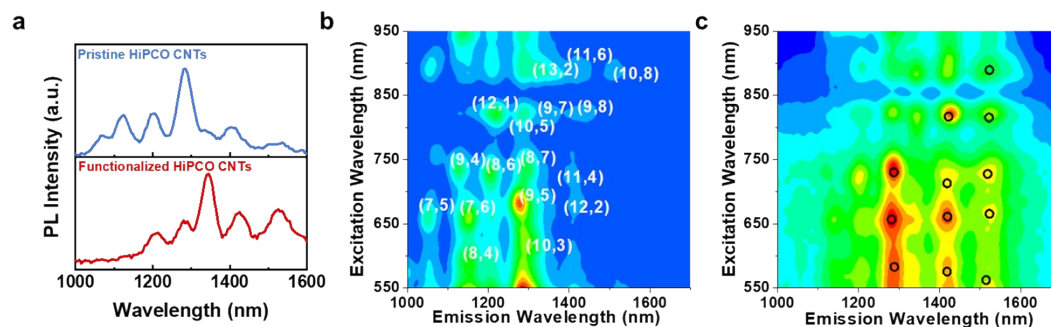


**Figure. S4** (a) and (b) are absorption spectra of SDS dispersed HiPCO SWCNTs without semiconductor purification and ultimately transposed into aqueous solution. After polymer separation, the metallic SWCNTs absorption peak between 400 and 600 nm disappears.



**Figure. S5.** The absorption spectra of SWCNTs with (10,5) tubes as the dominant chiral species in initial dispersion and  $H_2O$ .

To calculate the yield from the initial dispersion to the final in aqueous solution, the same volume of solvent was used to test the absorption spectra. The absorbance of Figure S1b is the actual value, which changed from 0.30 to 0.18, resulting in a final yield of 60%. The advantage of our method is that the multi-step cleaning of toluene and chloroform completely collects SWCNT precipitates. Only the final step of centrifugation in aqueous solution requires the removal of some nanotubes that are not stably coated by surfactants.



**Figure. S6** (a) PL spectra of HiPCO s-SWCNTs before and after introducing  $sp^3$  defects. (b) and (c) are PLE map of HiPCO s-SWCNTs before and after introducing  $sp^3$  defects.

- 1 Gu, J.; Han, J.; Liu, D.; Yu, X.; Kang, L.; Qiu, S.; Jin, H.; Li, H.; Li, Q.; Zhang, J., *Small* 2016, **12** (36), 4993-4999
- 2 Li, Y.; Zheng, M.; Yao, J.; Gong, W.; Li, Y.; Tang, J.; Feng, S.; Han, R.; Sui, Q.; Qiu, S.; Kang, L.; Jin, H.; Sun, D.; Li, Q., *Advanced Functional Materials* 2022, **32** (1), 2107119