## **Supporting Information**

# Key Factor in Enhancing Yield and Stability in Single-Chirality Carbon

## Nanotubes Extraction: Solvent Viscosity

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### 1. Experimental Section

### 1.1 Materials

The study was carried out using (6,5)-enriched CoMoCAT SWCNTs (Sigma Aldrich, product number: 773735. Raw HiPCO SWCNTs were purchased from Nanointegris Inc. and utilized without modification. The chemical reagents used in the experiment, such

as toluene, tetralin and trichloromethane, were procured from China National Pharmaceutical Group Chemical Reagent Co., Ltd., with a purity of analytical grade.

#### 1.2 Polymer synthesis

The polymers Poly[(9,9-dioctylfluorenyl-2,7-diyl)-alt-(6,6'-2,2'-bipyridine)] (PFO-BPy) was synthesized through Suzuki polymerization reactions.



Fig.S1 Schematic diagram of Suzuki Polycondensation (SPC).

PFO-BPy was synthesized according to a modified literature procedure Under argon atmosphere, a solution of 9,9-dioctylfluorene-2,7-diboronic acid bis(pinacol)ester(1) (642 mg, 1 mmol, 1 eq.), 6,6'-dibromo-2,2'-bipyridine(2) (314 mg, 1 mmol, 1 eq), Pd(AcO)2 (6 mg, 0.02 mmol, 0.02 eq), and tricyclohexylphosphine (12 mg, 0.04 mmol, 0.04 eq) in toluene (20 mL) was stirred and heated to 80 °C. After the mixture became clear, Et4NOH (2 mL) and deionized water (2 mL) were added. The solution was kept in the range of 80–85 °C with vigorous stirring under argon for 20 h. The end groups were capped by refluxing 6 h with monomer 1 (20 mg) and bromobenzene, respectively. After cooling, the resulting polymers were precipitated into methanol (200 mL) and filtered off. The product was dissolved in dichloromethane and washed three times with water. Then after removal of the solvent, the resulting polymers were received by precipitation in methanol. The resultant polymers were washed with acetone and dried under vacuum. The polymer was purified by soxlet extraction for 14 h using toluene and chloroform yielded higher molecular weight polymer with yields of 55%.

#### **1.2 Preparation of SWCNTs Dispersions**

1 mg of selected SWCNTs and 2 mg of polymer were separately weighed into glass vials. 2 mg polymer was dissolved in 5 ml of the selected solvent or solvent mixture. Polymer solution water bath ultrasound for 30 minutes in the next step, the polymer solution was transferred to a vial with pre-weighed SWCNTs. The solutions were ultrasonicated with a top-tip dispergator (Sonics VC500) for 1 h at an amplitude level of 30%, and then were centrifuged at 40 000 g for 1 h (Allegra X-22R centrifuge) to remove the bundles and insoluble materials. The supernatants were collected for follow-up experiment.

#### **1.3 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 arc lamp and a liquid-nitrogen-cooled InGaAs line camera from Horiba Inc.The atomic force microscope (AFM) images were characterized by a Dimension ICON with a tapping mode from Bruker. Nanoscope Analysis was used to analyze the morphology of AFM images.

#### **1.4 Fabrication of Monochiral SWCNT FETs**

FET devices with a microscale channel were fabricated on a silicon wafer with a 300 nm-thick thermal oxide layer. The supernatant prepared by diluting with toluene was then allowed to deposit on a silicon wafer for 4 hours. The deposited monochiral SWCNT films are used to make FET devices. Then FET devices with a channel length of 5 μm were fabricated using UV photolithography techniques. The source/drain electrodes were patterned by photolithography. And we use Oxygen plasma etching to remove SWCNTs out of the FET channel to prevent electric leakage. CLSM image of the devices was characterized by VX-250. The device's electronic performance was tested using a Keithley 4200 semiconductor parameter analyzer.

#### **1.5** Determination of the Concentration of (n, m) in Solution-state Samples

The number densities of different (n, m) species were determined according to the experimental absorbance and the estimated absorption cross section that was specific to each (n, m). The absorption cross section per atom,  $\sigma$  and the corresponding molar absorptivity,  $\varepsilon$  were calculated from the following relations.<sup>1</sup>

$$\sigma(\omega) = \frac{2.303 A(\omega)}{\iota \rho} \qquad \text{and} \qquad \varepsilon(\omega) = \frac{A(\omega)}{\iota c} \tag{1}$$

where  $A(\omega)$  is the resonant part of the frequency-dependent decadic absorbance,  $\iota$  is the optical path length,  $\rho$  the number density of carbon atoms.

$$\rho^{n,m} = \frac{N^{n,m}}{V_{eff}} \frac{\langle L \rangle^2}{\langle L \rangle} k^{n,m}$$
(2)

Where  $N^{n,m}$  is the number of (n,m) SWCNTs in effective probed volume  $V_{eff}$ ,  $k^{n,m}$  is the number of carbon atoms per unit length in the (n,m) structural species

By consulting literature, we found  $N^{6,5}$ = 1906 ± 60,  $k^{n,m}$  (88 400 atoms per µm for a (6,5) SWCNT) and (6,5) S11 peak absorbance and the cross section value of 2.54 × 10–17 cm2/C atom. Combining this result with the  $\rho^{6,5}$  value through eq 2, we determined the value of our effective volume,  $V_{eff}$  to be 14 pL. By substituting it into formula 1, we calculate the peak  $\varepsilon_{11}$  (0.55 (µg/ml)<sup>-1</sup>cm<sup>-1</sup>) for (6,5).<sup>2</sup> By deconvolution and the corresponding molar absorptivity of a given selected absorption spectrum, the concentration of chiral single-walled carbon nanotubes can be obtained

### 2. Characterization



Fig. S2 <sup>1</sup>H NMR spectrum of PFO-BPy synthesized in-house

	Density	Viscosity		Dielectric
Solvent			Polarity	constant
	(g/mL)	(mpa·s)		(-)
Decalin	0.880	3.40	0.015	2.2
p-xylene	0.857	0.65	0.074	2.3
Tetralin	0.974	2.20	0.086	2.8

**Table S1** Selected physicochemical parameters of applied solvents sorted in ascendingorder of Polarity.<sup>3,4</sup>

Toluene	0.867	0.59	0.099	2.4
m-xylene	0.868	0.62	N/A	2.7
o-xylene	0.879	0.81	N/A	2.6
chlorobenzene	1.106	0.75	0.188	5.7
THF	0.888	0.48	0.207	7.6
Chloroform	1.480	0.54	0.259	4.8
1,1,2-trichloroethane	1.435	1.52	0.296	7.3
1,2-dichloroethane	1.235	0.78	0.327	10.4



**Fig. S3** UV-Vis-NIR absorption spectra of CoMoCAT SG65i SWCNTs dispersed in sodium cholate aqueous solution.



Fig. S4 Schematic diagram of the preparation process for SWCNTs.

**Table S2** Effects of low-polarity solvents with similar densities on the sorting of (6,5)SWCNTs.

Solvent	Density	Concentration
	(g/mL)	(µg/mL)
p-xylene	0.857	0.98
toluene	0.867	0.56
m-xylene	0.868	1.22
o-xylene	0.879	1.89



**Fig. S5** (a) The influence of the SWCNTs: PFO-BPy weight ratio (in tetralin) on the yield and selectivity of extraction. (b)Excitation—emission photoluminescence maps of supernatants obtained using various amounts of PFO-BPy.



**Fig.S6** Normalized absorbance spectraof various cosolvents to tetralin on the CPE separation course



**Fig. S7** Absorption Spectra under Different Mixed Solvent Ratios: (a), (b), and (c) Correspond to  $\chi$ = 0.25,  $\chi$  = 0.50, and  $\chi$ = 0.75, Respectively.



**Fig. S8** PL excitation-emission maps of (6,5)-enriched CoMoCAT SWCNTs suspended with (a) tetralin only (b) tetralin: toluene=75:25 (c) tetralin: toluene=50:50



**Fig. S9** (a) Viscosity for toluene/tetralin binary mixtures at 298 K. <sup>5</sup> (b) Density for toluene/tetralin binary mixtures at 298 K.  $\chi$  represents the volume fraction of tetralin in a mixture of toluene and tetralin.



**Fig. S10** Deconvolution of optical absorbance spectra of SWCNTs suspended with (a) tetralin only and (b) toluene-tetralin mixture (v/v = 1:1).



**Fig. S11** SG65i-SWCNTs were separated by F8BT in Mixed tetralin: (a) Absorption spectra of (7,3) SWCNTs.

**Table S3** Comparison of the trade-off between the separation yield and purity of (6,5) SWCNTs dispersions harvested using conjugated polymer extraction with different methods.<sup>6–14</sup> The separation yield is express by concentration of (6,5) SWCNTs dispersions harvested. Loading factor is calculated by dividing the concentration of (6,5) SWCNTs dispersions harvested in  $\mu$ g/mL by the amount of polymer BPy used per milliliter of solution in mg Tradition stands for the standard method of sorting (6,5) SWCNTs. Mw represents the impact of different molecular weights on the isolation efficiency. Modification represents the modification of polymer. SFM is short for Shear Force Mixing. Enhancer represents the addition of molecular enhancers.

Method	References	Concentration (µg/ml)	Polymer content (mg/ml)	Loading factor (µg/ml∙mg)	Purity (%)
tradition	6	0.58	1.0	0.58	91
	7	1.28	2.0	0.63	99
Mw	8	4.35	1.3	3.26	93
modification	9	0.21	0.6	0.35	96
enhancer	10	9.98	1.1	9.07	86
	11	1.09	0.5	2.18	90
solvent	12	5.36	1.0	5.36	86
	13	2.58	1.2	2.15	83
	6	1.09	1.0	1.09	88
	6	0.58	1.0	0.58	86
	6	0.42	1.0	0.42	97
SFM	14	5.81	0.5	11.62	84
this work		11.25	0.4	28.12	85
		5.82	0.4	14.55	91



Fig. S12 Atomic force microscopy (AFM) images of (6,5) SWCNT films deposited from (a) toluene ( $\chi$ =0) and (b) mixed solvent ( $\chi$ =0.5)



**Fig. S13** AFM images of (6,5) SWCNT networks deposited for 0.5 and 4 hours using (a) toluene only (b) toluene-tetralin mixture (v/v = 1:1) (c) tetralin only.



**Fig. S14** Fig. S14 Transfer characteristics of (6,5) SWCNT FETs with channel length/width of 5  $\mu$ m/10  $\mu$ m, Vds=-1: (a) and (c): toluene (b)and(d) toluene-tetralin mixture (v/v = 1:1)

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