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Supplementary material

Change in chirality of semiconducting single-walled carbon nanotubes can overcome anionic surfactant stabilisation: a systematic study of aggregation kinetics

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Table S1. Properties of surfactants used

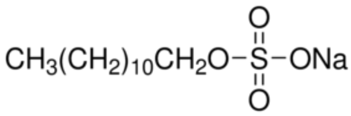
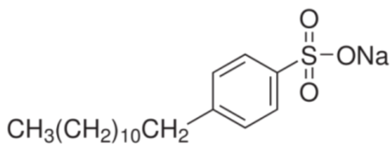
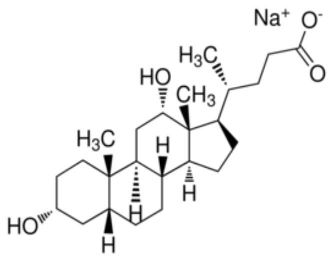
Chemical name	Chemical formula	Structure	MW (g mol^{-1})	CMC (mg mL^{-1})
SDS (sodium dodecyl sulfate)	$NaC_{12}H_{25}SO_4$		288.4	2.02–2.90
SDBS (sodium dodecyl benzenesulfonate)	$NaC_{18}H_{29}SO_4$		348.48	0.73–1.40
SDOCO (sodium deoxycholate)	$NaC_{24}H_{39}O_4$		414.6	0.83–2.48

Table S2. Mass concentration of surfactant-modified SWNTs

SWNT sample	Surfactant	Mass conc. (mg L^{-1})		
		Initial	After 24 h	After centrifugation
SG65	SDS	109	96.69 ± 0.02	31.82 ± 0.04
	SDBS	102	90.69 ± 0.48	46.25 ± 0.02
	SDOCO	104	93.59 ± 0.06	47.20 ± 0.01
SG76	SDS	103	85.34 ± 0.19	30.86 ± 0.22
	SDBS	106	98.24 ± 0.10	40.44 ± 0.10
	SDOCO	107	96.93 ± 0.38	59.72 ± 0.16

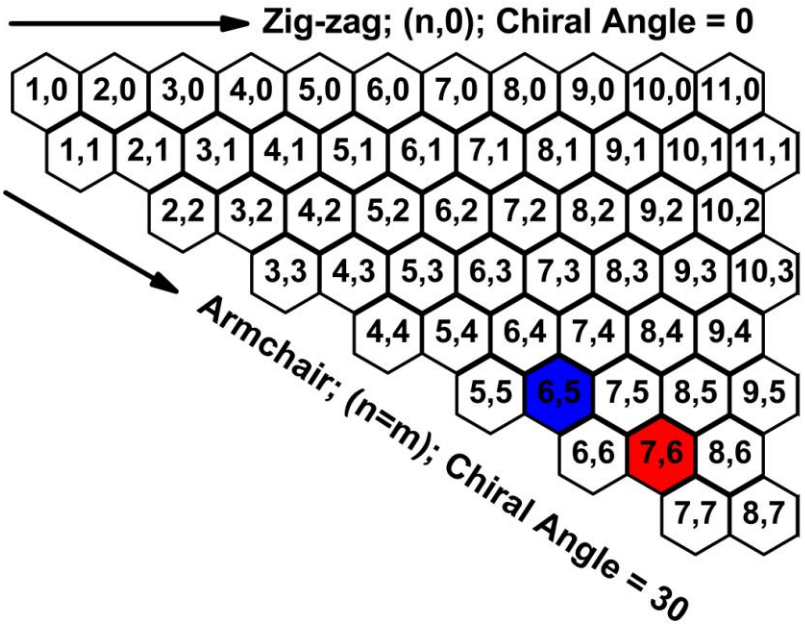


Fig. S1. Chirality chart of SWNTs. Chiral indices of (6, 5) and (7, 6) are shown through colour coding: blue and red respectively. The two arrows represent boundaries of atomic arrangements; horizontal arrow is the zig-zag and angular arrow is the armchair extreme for chiral arrangements.

Method for AFM

For AFM, SWNTs (0.5 mg) added to SDS solution (1 %, 15 mL) were sonicated for 30 min (at 50 % amplitude) with an ultrasonic dismembrator (Misonix S-4000). The suspensions were then kept at room temperature for 24 h. To ensure homogeneous distribution of the tubes, spin-coating was carried out at 500–700 rpm for 30–60 s. SWNTs (60–80 μL) were added dropwise to optically smoothed 1 × 1-cm silicon wafers. Prior to addition of the SWNTs, the wafer sections were cleaned with methanol and deionised water, followed by drying with argon and heating for 3 min at 100 °C. After addition of the SWNT suspension, the wafers were dried for 1 min to evaporate residual liquid. AFM imaging was performed using Nanoscope IIIA (Veeco Technologies, Plainview, NY). A silicon AFM tapping tip (NanoDevices Inc., Santa Barbara, CA) was used to obtain the morphological information from the nanotube-coated wafers.

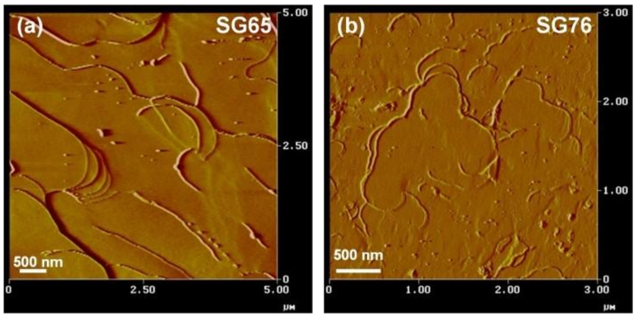


Fig. S2. Representative AFM images of functionalised (a) SG65; and (b) SG76 SWNTs.

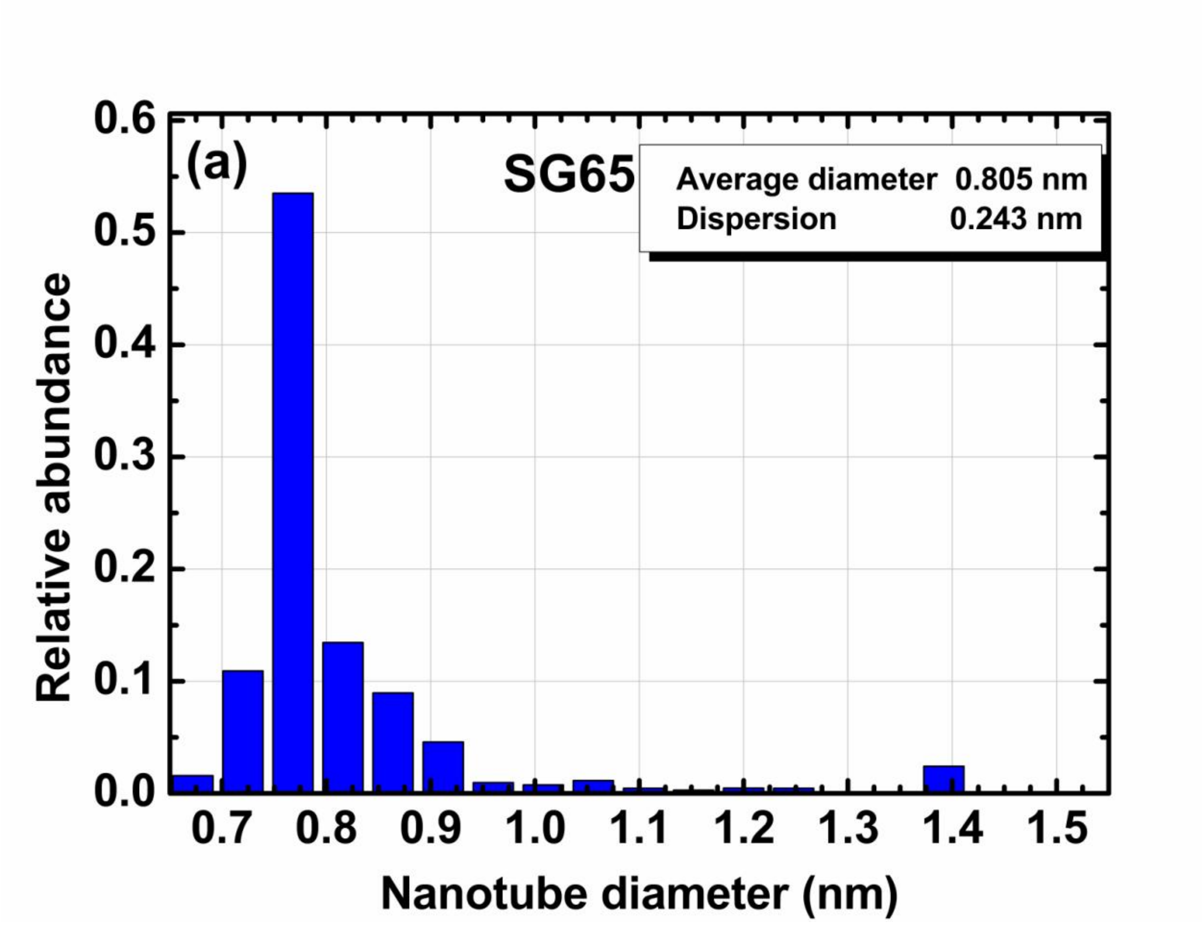


Fig. S3. Diameter distribution of (a) SG65; and (b) SG76 SWNTs from fluorescence analysis.

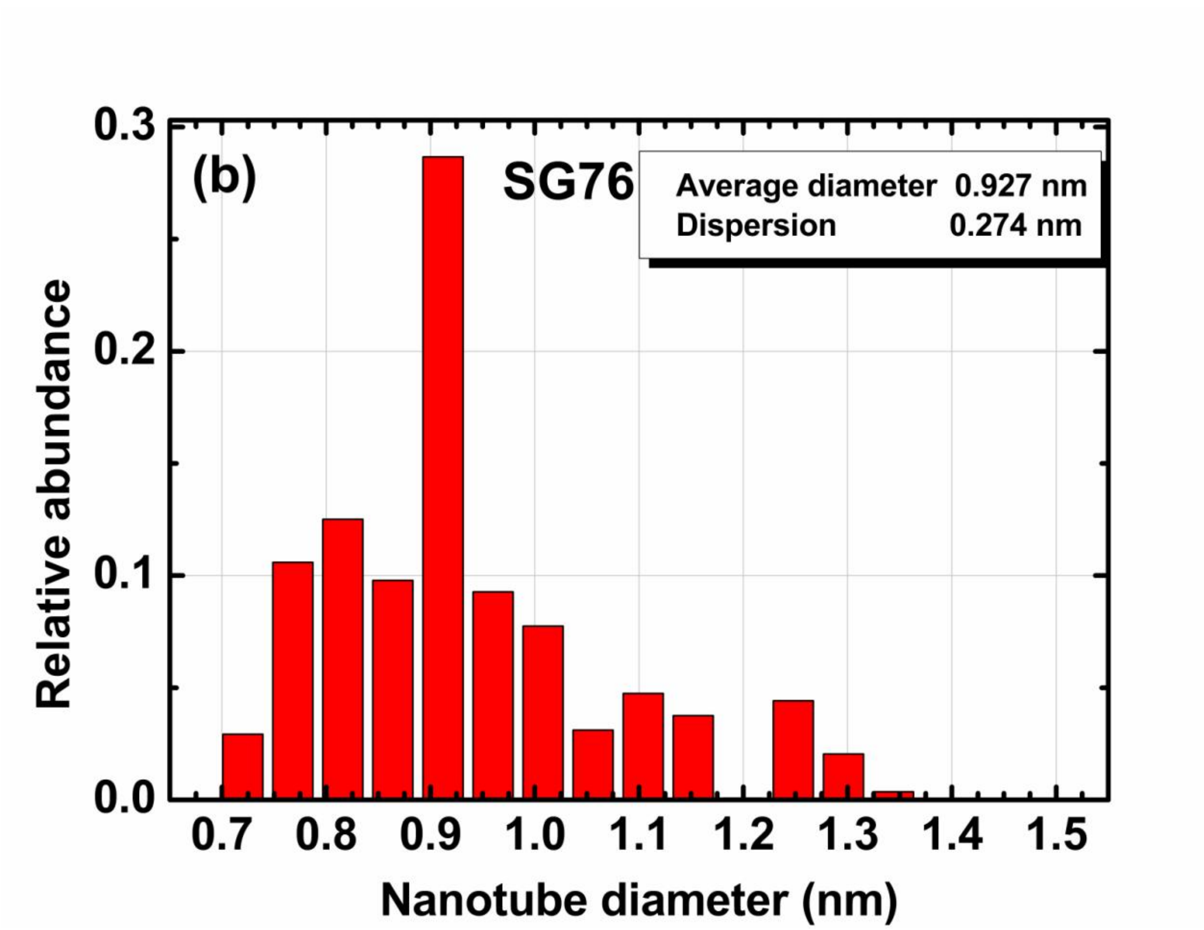

(b)
SG76
Average diameter 0.927 nm
Dispersion 0.274 nm
Relative abundance
0.0
0.1
0.2
0.3
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
1.5
Nanotube diameter (nm)

Fig. S3. *(Cont.)*

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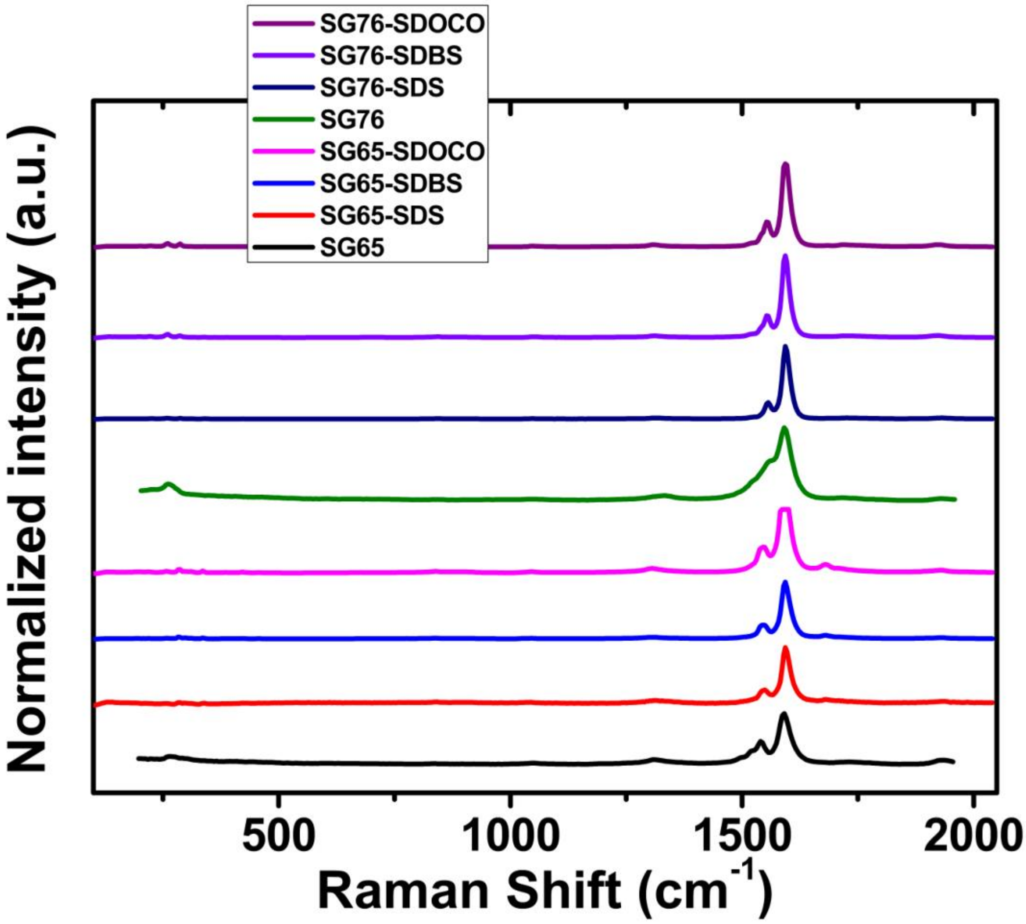
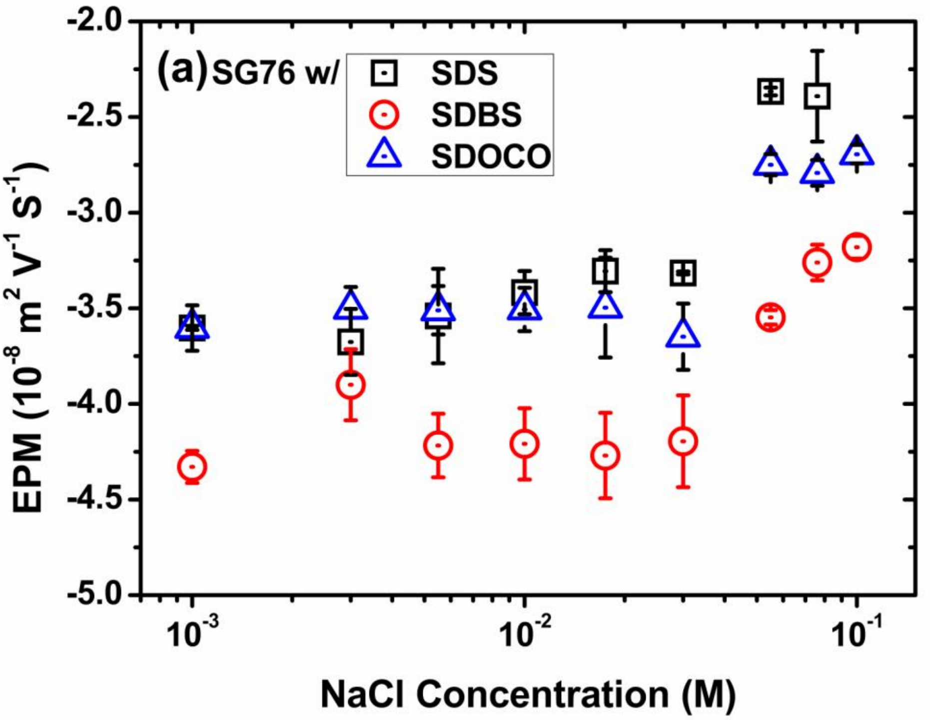


Fig. S4. Raman spectra of pristine and surfactant-modified SWNTs presenting the higher Raman frequency regions with defect representing 'D' band (near 1320 cm^{-1}) and graphitic signature containing 'G' band (near 1592 cm^{-1}). Intensity for each spectrum is relevant to that specific measurement and shows relative D/G intensities for that specific case. D/G ratios calculated from respective Raman spectrum are shown in Table S3.

Table S3. Calculated D/G ratio from Raman spectra

SWNT sample	D/G ratio	SWNT sample	D/G ratio
SG65-Pristine	0.24 ± 0.01	SG76-Pristine	0.12 ± 0.01
SG65-SDS	0.04 ± 0.01	SG76-SDS	0.06 ± 0.01
SG65-SDBS	0.07 ± 0.01	SG76-SDBS	0.07 ± 0.01
SG65-SDOCO	0.14 ± 0.01	SG76-SDOCO	0.08 ± 0.01



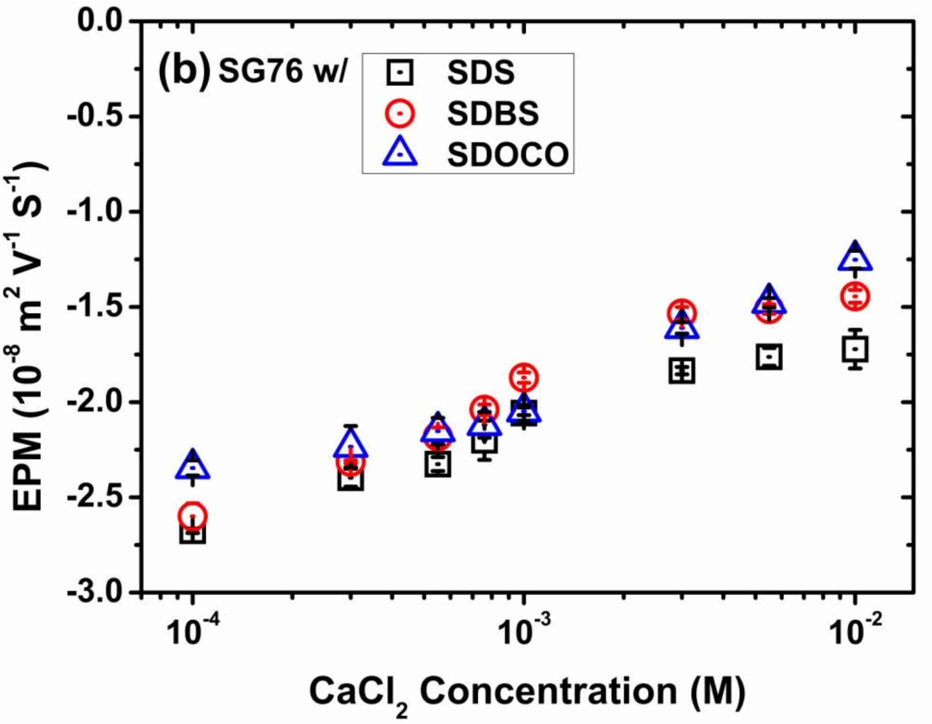


Fig. S5. Electrophoretic mobility (EPM) of SG76 SWNTs as a function of (a) NaCl; and (b) $CaCl_2$ salt concentration. At least three separate experiments were performed under each set of conditions and data presented here are mean of three independent experiments with one standard deviation. Measurements were carried out at a pH of ~6.5 and a temperature of 20 ± 0.5 °C.

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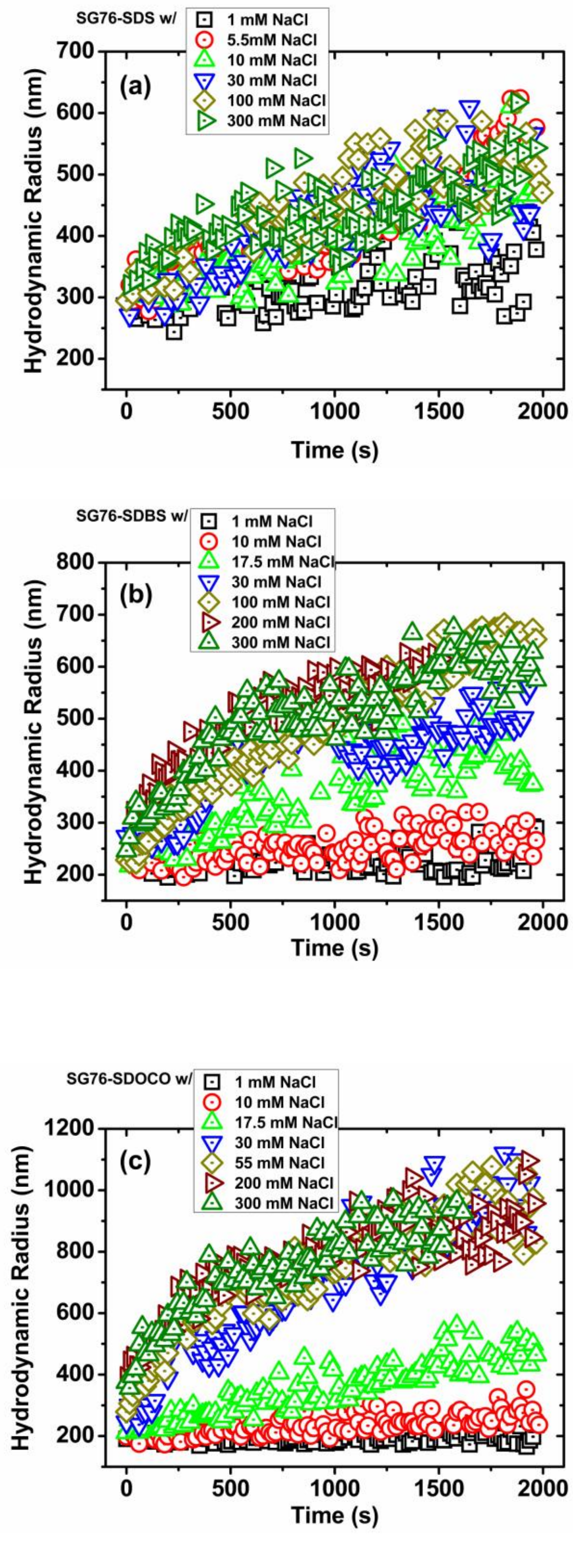

Fig. S6. Aggregation profiles of (a) SDS-, (b) SDBS- and (c) SDOCO-modified SG76 SWNTs under range of NaCl electrolyte concentrations. Aggregation experiments were conducted at a temperature of 20 ± 0.5 °C and at least duplicate samples were tested to obtain significant reproducibility.

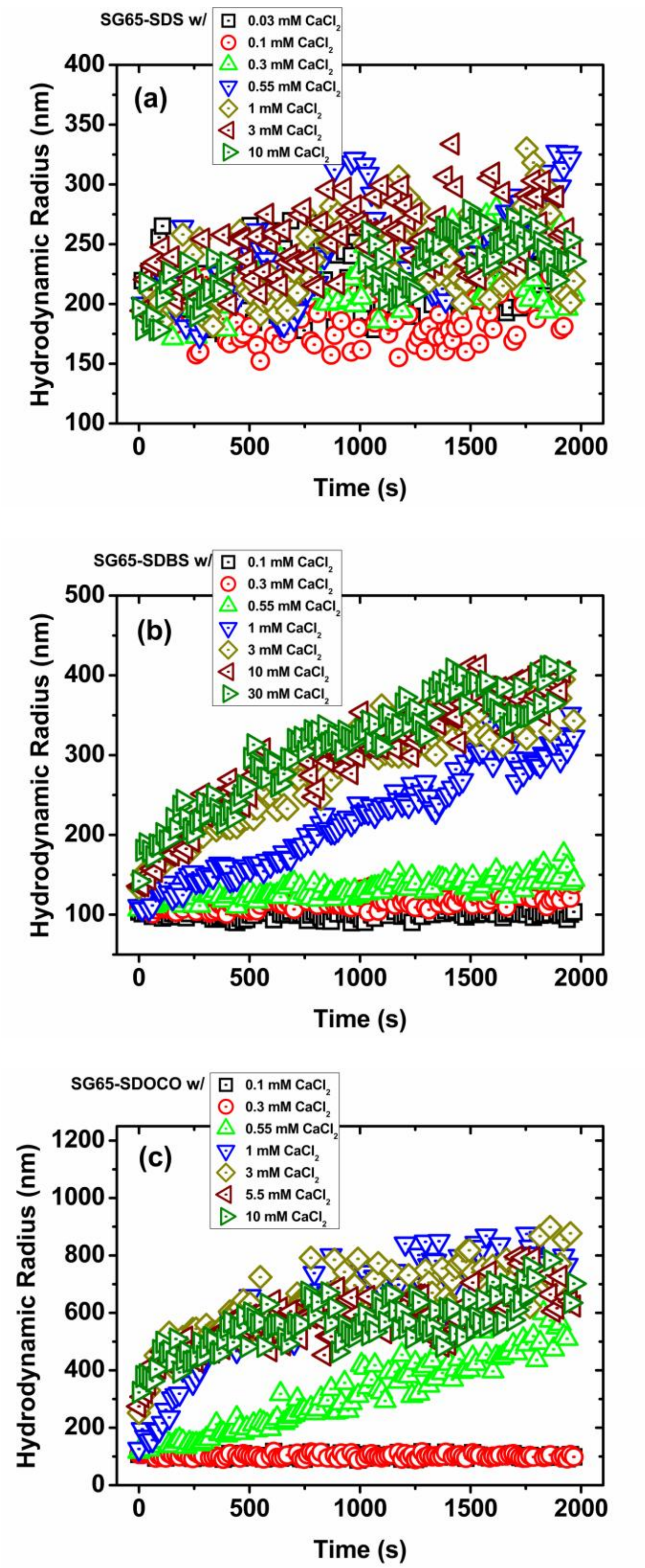

Fig. S7. Aggregation profiles of (a) SDS-, (b) SDBS- and (c) SDOCO-modified SG65 SWNTs range of $CaCl_2$ electrolyte concentrations. Aggregation experiments were conducted at a temperature of 20 ± 0.5 °C and at least duplicate samples were tested to obtain significant reproducibility.

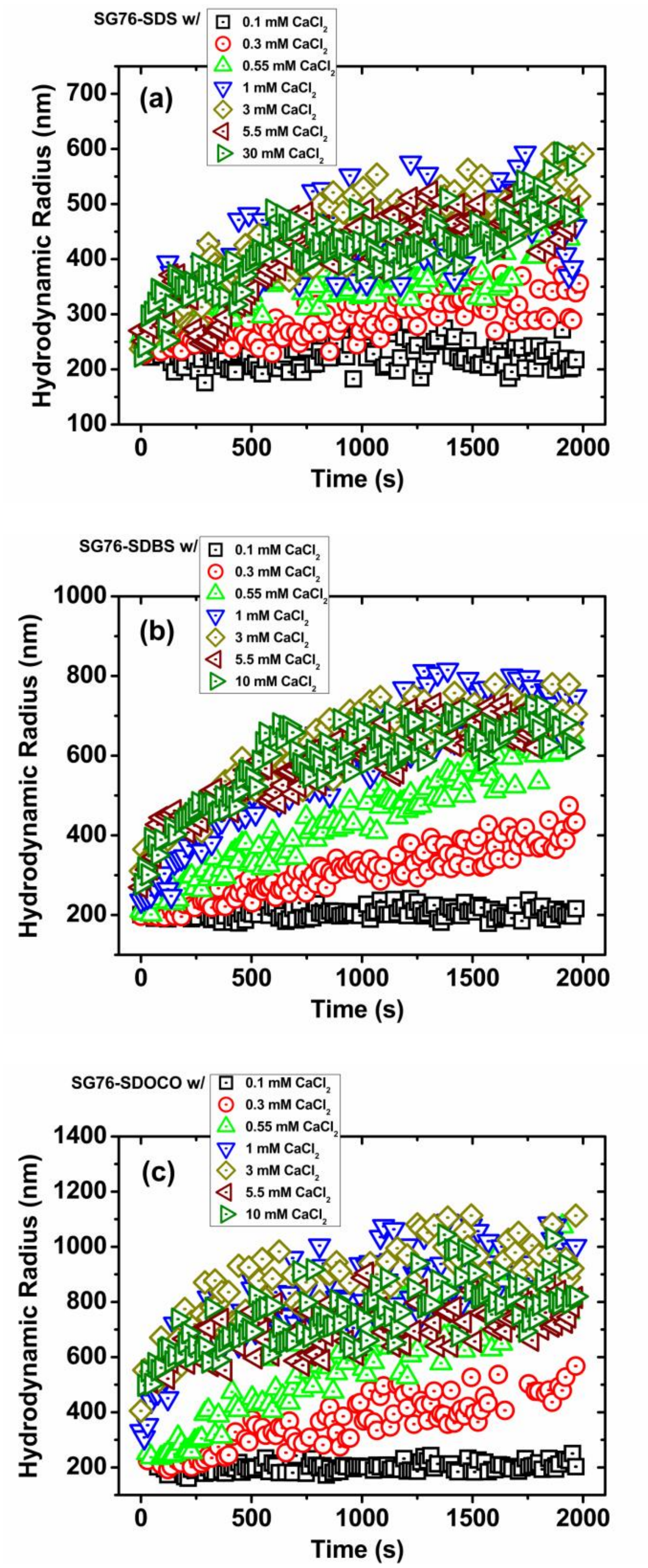

Fig. S8. Aggregation profiles of (a) SDS-, (b) SDBS- and (c) SDOCO-modified SG76 SWNTs under range of $CaCl_2$ electrolyte. Aggregation experiments were conducted at a temperature of 20 ± 0.5 °C and at least duplicate samples were tested to obtain significant reproducibility.

Table S4. Initial aggregation rate of SWNTs in absence and presence of SRHA under 10 mM NaCl, and 7 mM NaCl plus 1 mM $CaCl_2$ electrolyte conditions (data for Fig. S9)

Electrolyte	SWNT sample	SDS	SDBS	SDOCO
10 mM NaCl	SG65	0.148 ± 0.019	0.061 ± 0.004	0.101 ± 0.008
	SG65 with SRHA	0.030 ± 0.002	0.015 ± 0.002	0.017 ± 0.013
	SG76	0.108 ± 0.034	0.469 ± 0.066	0.059 ± 0.008
	SG76 with SRHA	0.002 ± 0.005	0.056 ± 0.006	0.017 ± 0.003
7 mM NaCl + 1 mM $CaCl_2$	SG65	0.202 ± 0.022	0.072 ± 0.004	0.712 ± 0.148
	SG65 with SRHA	0.007 ± 0.003	0.003 ± 0.002	0.008 ± 0.002
	SG76	0.111 ± 0.015	0.641 ± 0.124	0.883 ± 0.047
	SG76 with SRHA	0.039 ± 0.005	0.011 ± 0.005	0.005 ± 0.002

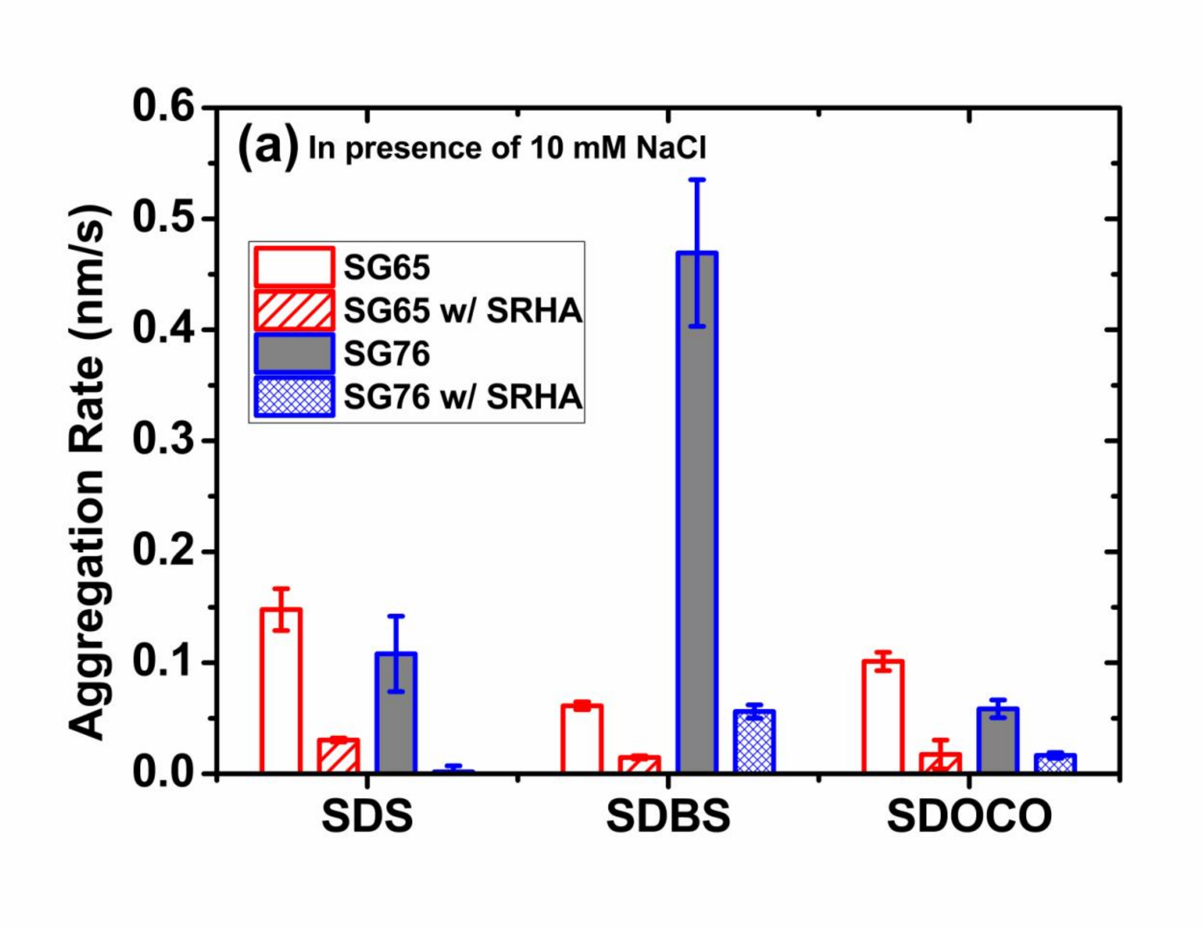

Fig. S9. Initial aggregation rate plots of SWNTs in the absence and presence of 2.5 mg TOC L^{-1} Suwannee River humic acid (SRHA) as function of (a) 10 mM NaCl; and (b) 7 mM NaCl + 1 mM $CaCl_2$. The rates are calculated from corresponding aggregation profiles. All the aggregation experiments were conducted at a temperature of 20 ± 0.5 °C and at least duplicate samples were tested to obtain significant reproducibility. (TOC, total organic carbon.)

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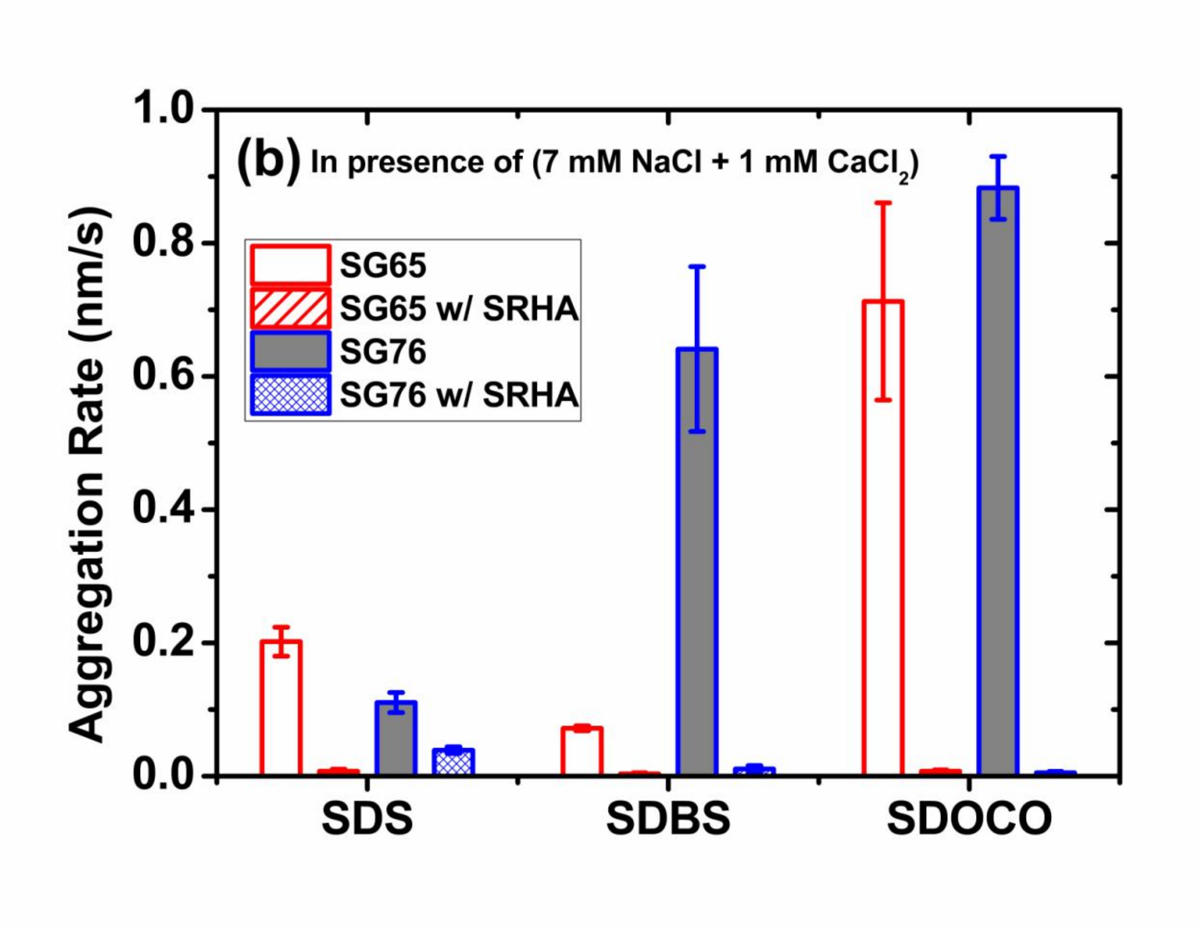

Fig. S9. *(Cont.)*