

Supporting Information for

**Selective Desorption of High-Purity (6,5) SWCNTs from Hydrogels through Surfactant Modulation**

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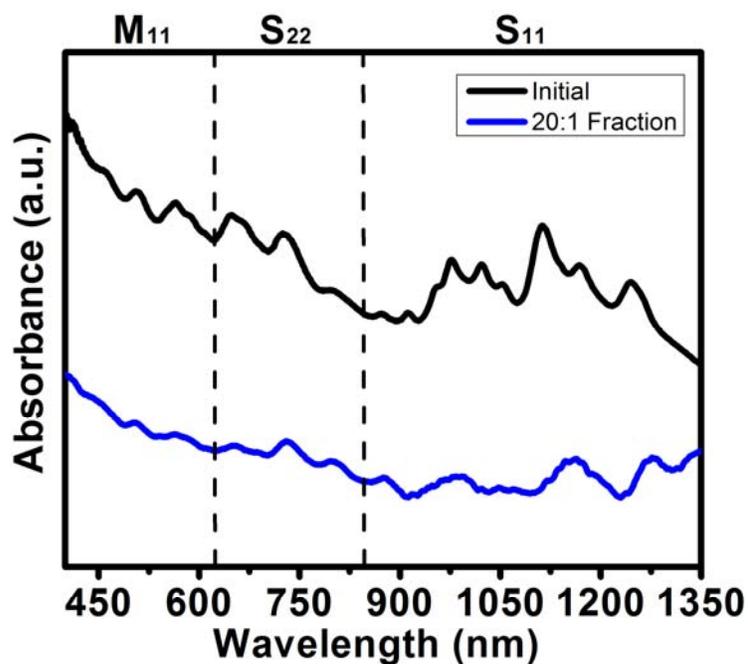
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**Materials.** Nanopure water (18 mΩ) was used in all experiments. Both SDS ( $\geq 99\%$ ) and DOC ( $\geq 97\%$ ) were purchased from Sigma-Aldrich and used as received. HiPco SWCNTs were obtained from Rice University (HPR 164.1) and used as received. The hydrogel (6FF) was manufactured by GE Healthcare and purchased directly from GE.

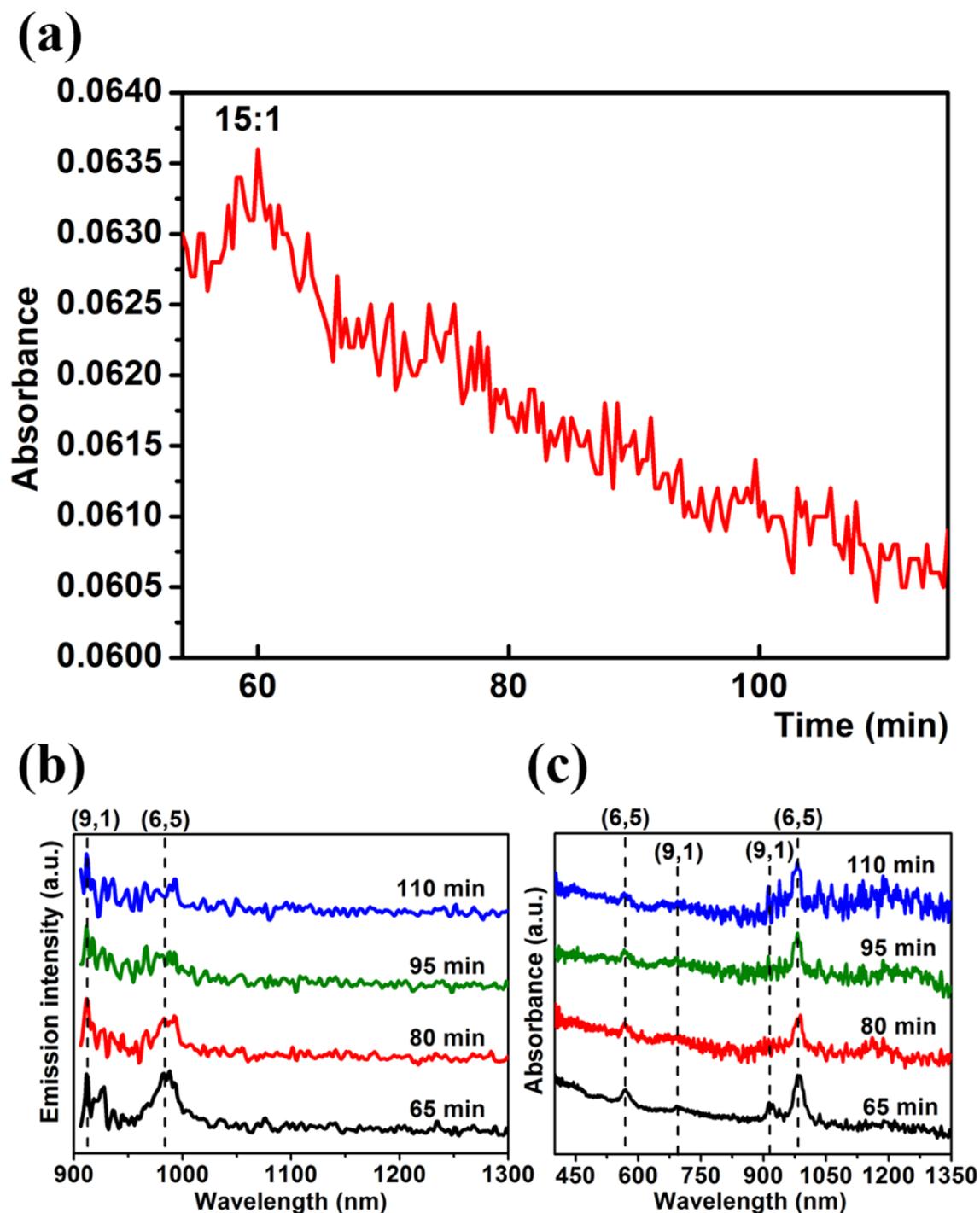
**Aqueous Suspension Preparation.** Aqueous suspensions of SWCNTs were prepared by mixing 30–40 mg of raw SWCNT powder (HPR 164.1) with 150 mL of a 35.0 mM SDS solution in Nanopure water. This solution was mixed at 8000 rpm (IKA T-25 Ultra-Turrax) for 40 min. After homogenization, the solution was allowed to rest for 15 min before cup horn ultrasonication (120 W, Misonix S3000) to aid dispersion. The ultrasonication step was repeated a total of three times to ensure a well-dispersed suspension. The solution was then ultracentrifuged for 4 h at 20 000 rpm (53 000g) to remove metallic catalysts, amorphous carbon, and SWCNT bundles from solution (Beckman Coulter Optima L-80K, SW-28 rotor).

**Column Experiments.** The single column experiments were completely automated (Chromleon software), allowing for sample injection, elution gradients, and real-time fraction characterization using an HPLC pump and fluorometer. Sample injection and binary gradient elution were controlled by an HPLC pump (Ultimate 3000, Dionex) with a flow rate of 1 mL/min. The low-pressure chromatography column (Bio-Rad) was made of glass and had an inner diameter of 1.5 cm. The column was packed with 5 mL of agarose beads (Sephacrose 6FF) that typically resulted in a column height of 3 cm. An Econo flow adapter (Bio-Rad) connected the column to the HPLC pump. The column and eluents were submerged in a water bath and chilled to 10, 15, or 20 °C. A typical experimental sequence consisted of first stabilizing the column with four column-volumes (CV) of 35.0 mM SDS solution. One-fifth of a CV of the initial suspension was then injected into the column. The metallic SWCNT fraction was collected first by elution with SDS. After removing the metallic fraction, different ratios of SDS/DOC co-surfactant solution were used to modulate the surface properties of the semiconducting SWCNTs adsorbed onto the hydrogel. Collected fractions were characterized by absorption (1.0 cm path) and fluorescence spectroscopy (1.0 cm path) on an Applied NanoFluorescence Nanospectralyzer (Houston, TX) with excitation from 662 and 784 nm diode lasers. Effluent from the column was continuously characterized in situ by use of a flow cell from Starna Cells. Typically, absorption spectra were taken every 20 s while the effluent flowed through the cell. Elution profiles of SWCNTs released from the column

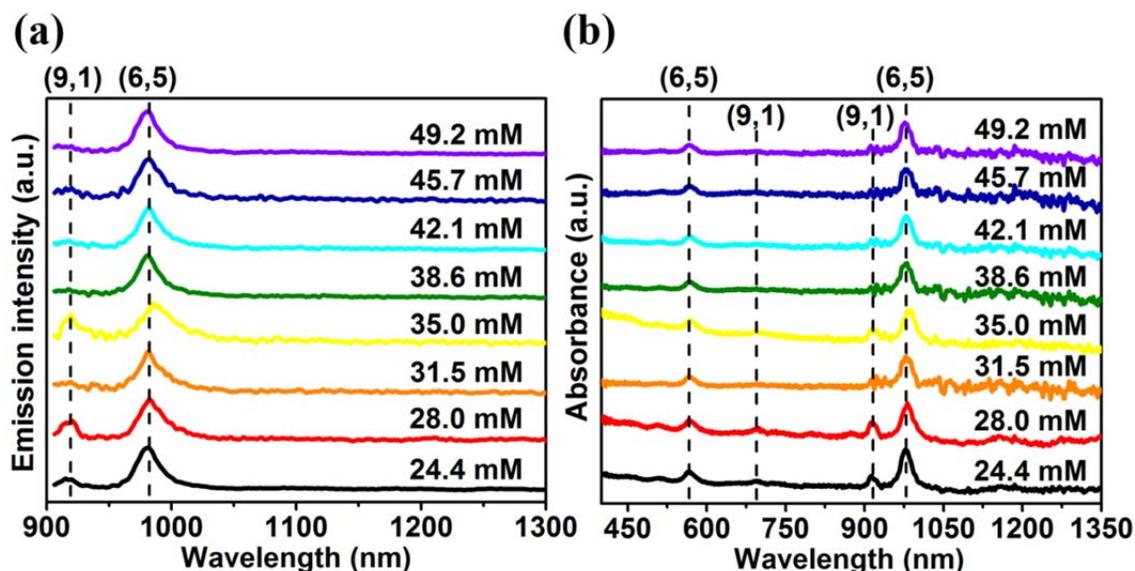
were estimated by use of absorbance values at 626 nm to account for the presence of both metallic and semiconducting SWCNT species. A Bio-Rad fraction collector (Model 2110) captured samples every 1.5 CV during elution. The purity of each  $(n,m)$  fraction was computed as the ratio of the area of the dominant peak to the sum of the areas of all peaks.



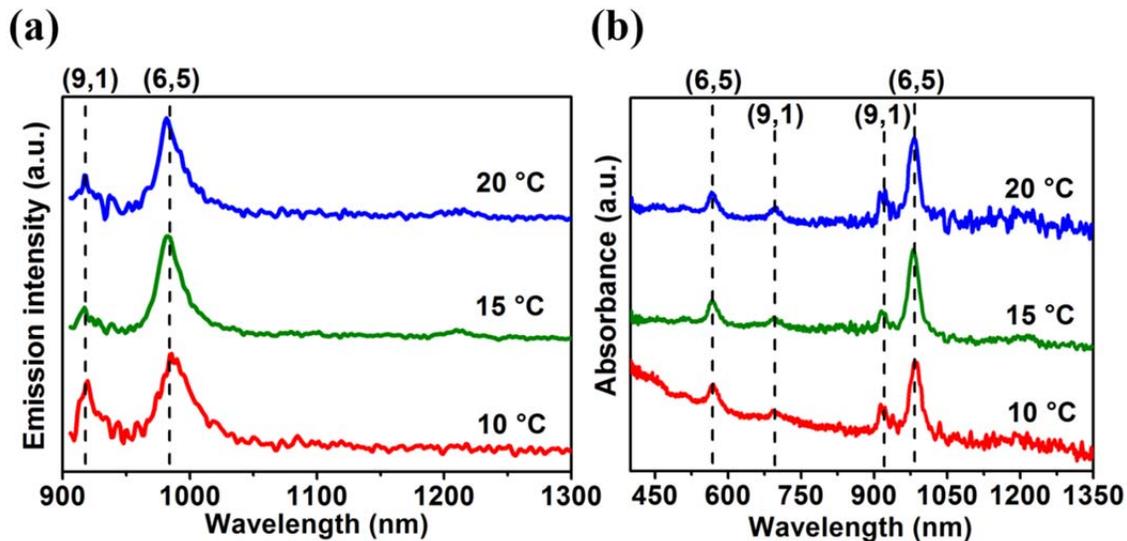
**Figure S1.** Normalized absorbance spectra ( $\lambda = 626$  nm) for the initial suspension and effluent collected with SDS:DOC ratio of 20:1. Note: The NIR region of the 20:1 fraction curve has been smoothed to leave out the noise that is caused by dilution. Spectra of the initial and 20:1 fraction have been slightly offset for visual clarity.



**Figure S2.** (a) Elution curve of SWCNTs suspended in 35.0 mM SDS with Sepharose 6 FF as the stationary phase. The elution curve is presented in terms of absorbance of effluent normalized by absorbance of initial suspension ( $\lambda = 626$  nm). Note that (6,5) SWCNTs are continuously eluted but the concentration falls quickly. (b) Fluorescence spectra (excited at 784 nm) of s-SWCNTs fractions collected during elution with SDS:DOC ratio of 15:1 at 15 min time intervals. (c) Corresponding absorbance spectra of the selectively separated s-SWCNTs fractions.



**Figure S3.** (a) Fluorescence spectra (excited at 662 nm) of s-SWCNTs fractions collected during elution with SDS:DOC co-surfactant solution at different background SDS concentrations between 24.4 and 49.2 mM. All the effluents were collected at 10 °C with an elution interval of 15 min. (b) Corresponding absorbance spectra of the selectively separated s-SWCNTs fractions.



**Figure S4.** (a) Fluorescence spectra (excited at 784 nm) of s-SWCNTs fractions collected during elution with an SDS:DOC ratio of 15:1 at temperatures of 10, 15, and 20 °C. (b) Corresponding absorbance spectra of the selectively separated s-SWCNTs fractions.