Supporting Information

Purification of Single-Wall Carbon Nanotubes by Controlling the Adsorbability onto Agarose Gels Using Deoxycholate

*Atsushi Hirano,[†,‡] Takeshi Tanaka,[†] Yasuko Urabe,[†,‡] Hiromichi Kataura *[,†,‡]*

† Nanosystem Research Institute, National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki 305-8562, Japan. ‡ JST, CREST, Kawaguchi, Saitama, 332-0012, Japan.

E-mail: h-kataura@aist.go.jp

* To whom correspondence should be addressed: Nanosystem Research Institute, National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki 305-8562, Japan. Tel.: +81-29-861-2551, Fax: +81-29-861-2786, E-mail: h-kataura@aist.go.jp

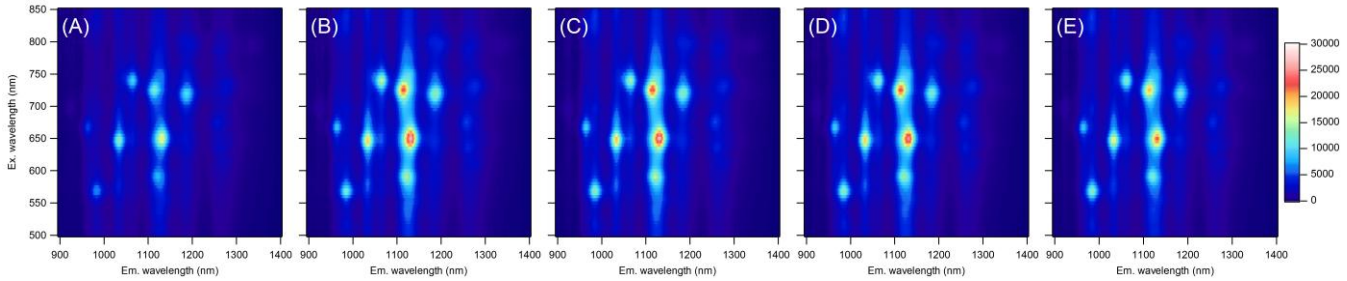

Figure S1. Fluorescence spectra of the SWCNTs dispersed at 0.05% (A), 0.1% (B), 0.25% (C), 0.5% (D), and 1% (E) DOC.

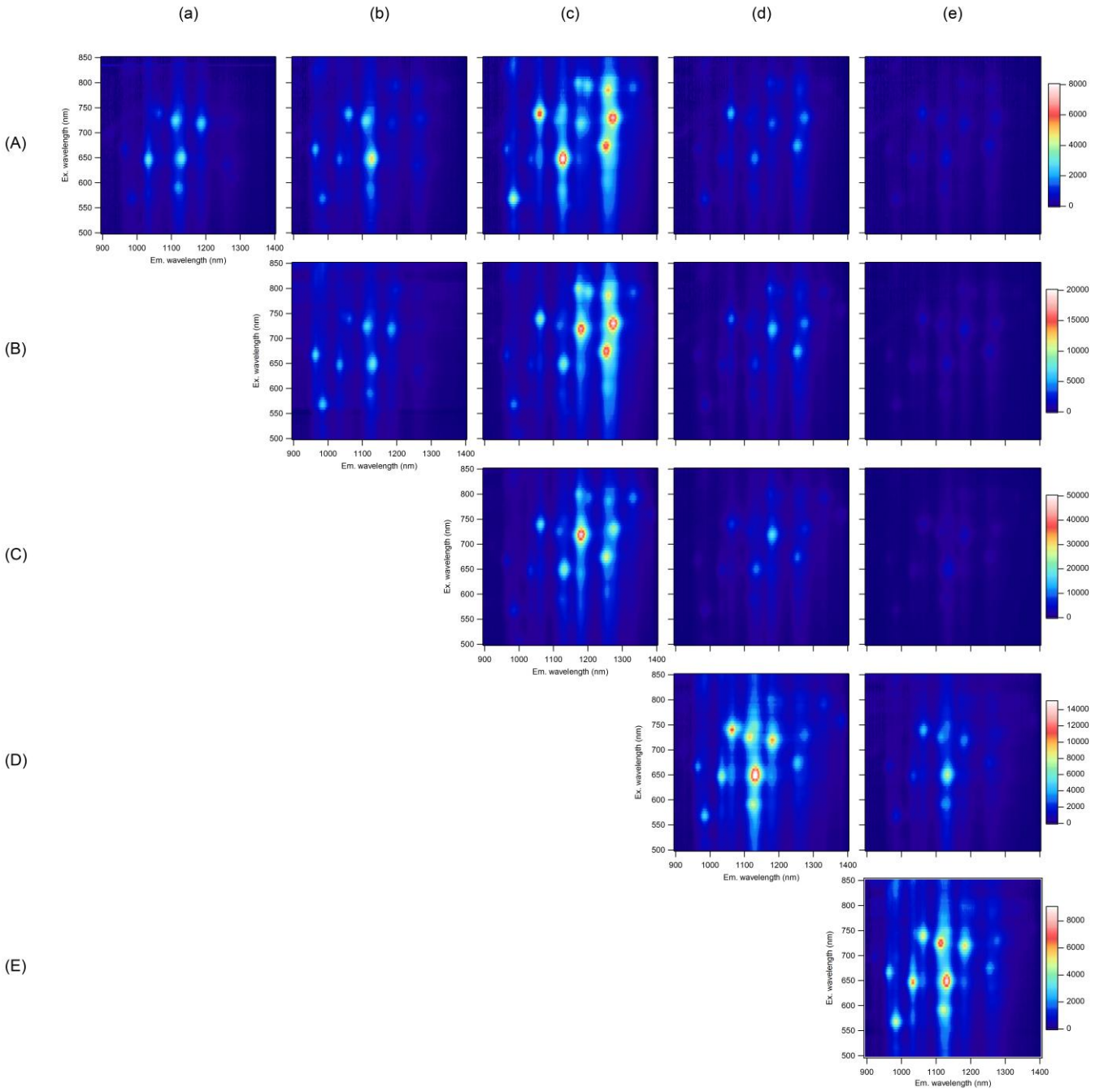

Figure S2. Fluorescence spectra of the SWCNTs obtained by adsorption onto agarose in 0.05% (row A), 0.1% (row B), 0.25% (row C), 0.5% (row D), and 1% (row E) DOC and subsequent stepwise elution with 0.1% (column a), 0.25% (column b), 0.5% (column c) 1% (column d), and 2% (column e) DOC.

Metal/semiconductor separation of SWCNTs using Sephacryl.

Metal/semiconductor separation of the SWCNTs was performed with Sephacryl in the open column, which was based on the following method. The SWCNTs collected from the supernatant of the dispersed solution, which was obtained by ultrasonication at 20 W cm^{-2} for 1 h and subsequent ultracentrifugation at 210,000 × *g* for 1 h in the presence of 0.5% SDS, were applied to the top of the column containing ca. 30 mL Sephacryl in 0.5% SDS. Metal-rich SWCNTs were obtained as the first flow-through fraction by the addition of 15 mL of 0.5% SDS, which shows the characteristic absorption spectrum of metallic SWCNTs (Figure S3). The subsequent addition of 0.5% SDS allowed the other unadsorbed SWCNTs to flow through the column, which was obtained as the second flow-through fraction. The spectrum for the second flow-through fraction was relatively broader than that for the first flow-through fraction, indicating that the purity of the metallic SWCNTs in the second flow-through fraction was lower than that of the metallic SWCNTs in the first flow-through fraction. Additionally, 1% SDS allowed the remaining metallic SWCNTs to be eluted. Subsequently, 25 mL of 1% DOC was added into the column, leading to the elution of the adsorbed SWCNTs. The solution obtained as the first eluate showed the characteristic absorption spectrum of semiconducting SWCNTs. The subsequent addition of 1% DOC allowed the other adsorbed SWCNTs to be eluted, which were obtained as the second eluate. The absorbance of the S_{11} and S_{22} bands for the second eluate was relatively lower than that of the bands for the first eluate, indicating that the purity of the semiconducting SWCNTs in the second eluate was lower than that of the semiconducting SWCNTs in the first eluate. Thus, high-purity metallic and semiconducting SWCNTs were obtained from the first flow-through fraction and first eluate, respectively. Nevertheless, the first flow-through fraction contained some impurities such as amorphous carbon or bundled SWCNTs, as evidenced by the broad absorption observed in the wavelength range. Thus, in the present study, the first flow-through fraction was used as the unpurified sample, as shown in Figure 6.

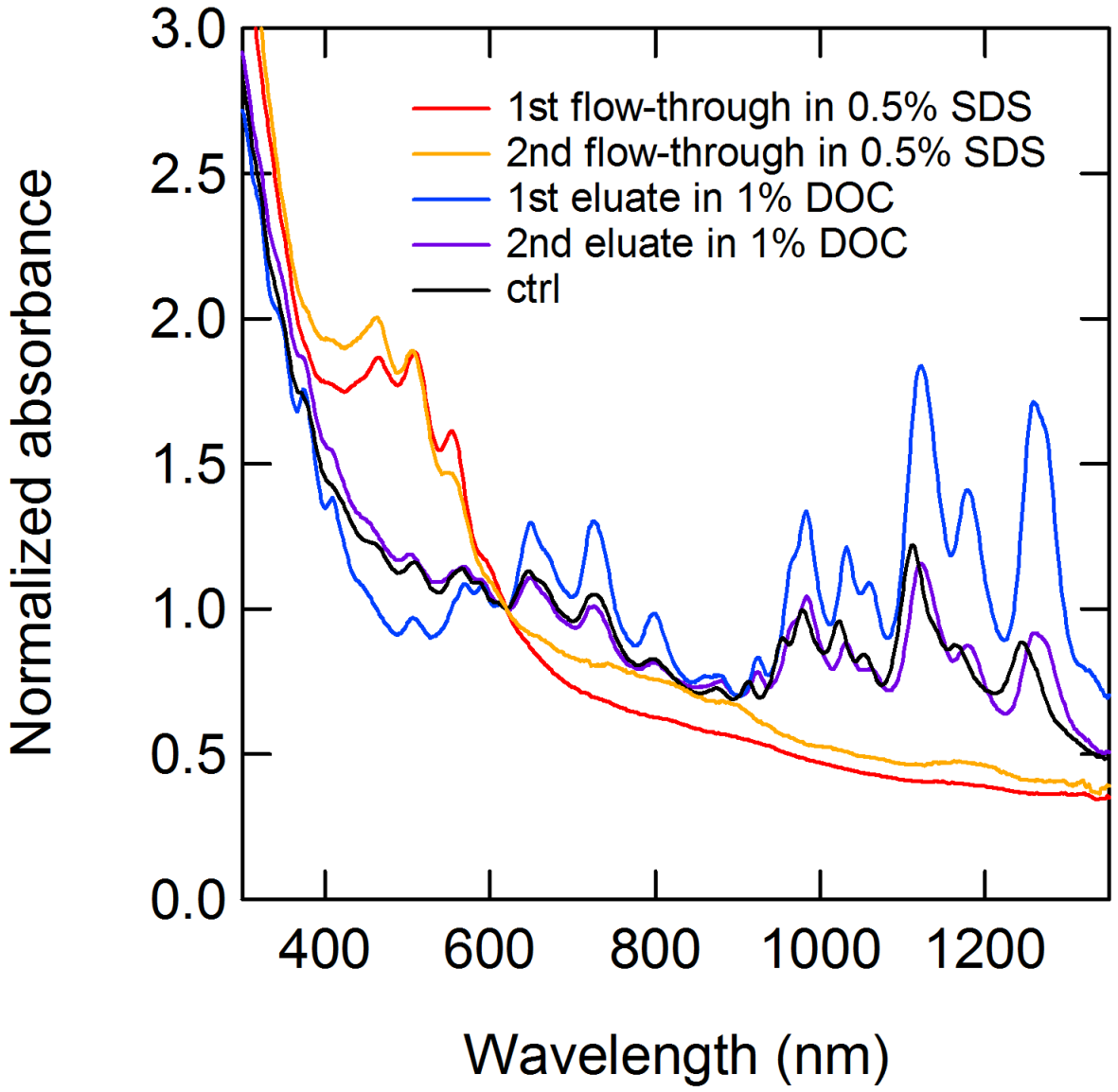

Figure S3. Absorption spectra, normalized at 620 nm, of the SWCNTs obtained from each fraction of the metal/semiconductor separation.

Fits to the absorption spectra

The fitting function consisted of a sum of Lorentzian peaks was used to fit the absorption spectra after subtraction of the background from the original normalized spectra using a polynomial function. Figure S4A,B shows the fits to the absorption spectra of the unpurified and purified metallic SWCNTs, respectively. Amplitude of representative peak was exhibited in Table S1. Amplitude for the purified metallic SWCNTs was higher than that for the unpurified species, also suggesting the removal of impurities by the agarose gel.

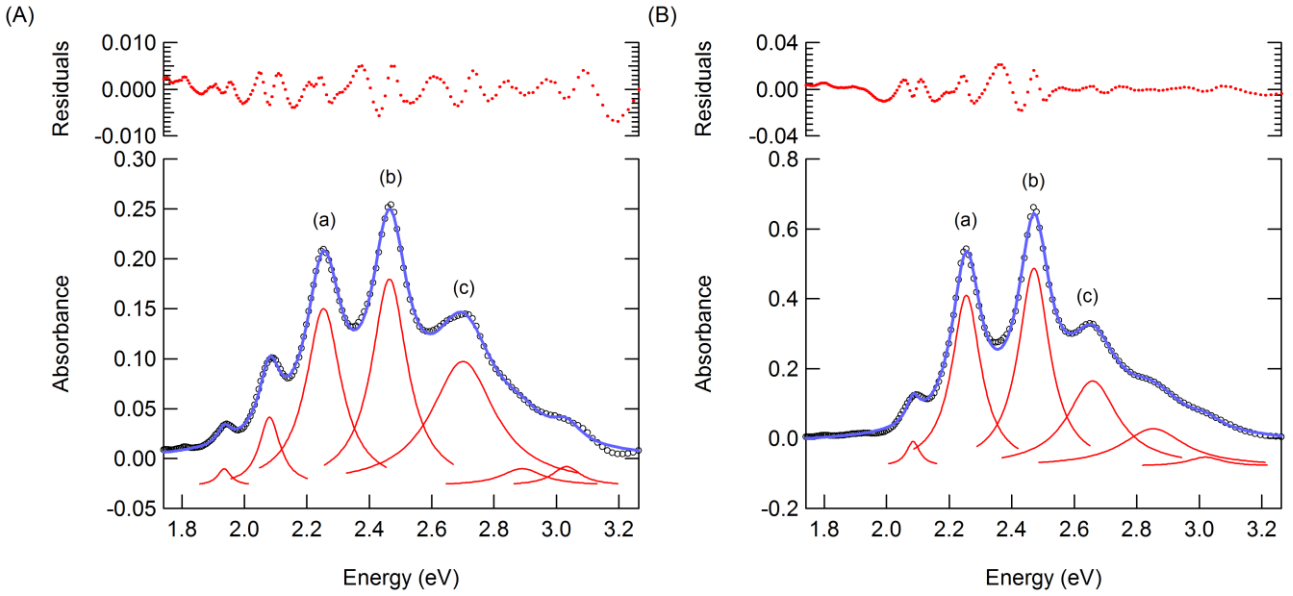

Figure S4. Absorption spectra (open circles) and their fits (purple lines) to a sum of Lorentzian peaks (red lines) for unpurified (A) and purified (B) SWCNTs.

Table S1. Amplitude and position of the representative peaks in Figure S4.

peak	unpurified SWCNTs		purified SWCNTs	
	amplitude	position (eV)	amplitude	position (eV)
a	0.18	2.25	0.49	2.25
b	0.21	2.46	0.57	2.47
c	0.12	2.70	0.24	2.66