

Enrichment Mechanism of Semiconducting Single-walled Carbon Nanotubes by Surfactant Amines

Sang-Yong Ju,[†] Marcel Utz,^{†,‡,‡} and Fotios Papadimitrakopoulos^{,†,§}*

Contribution from the Nanomaterials Optoelectronics Laboratory (NOEL), Polymer Program, Institute of Materials Science, University of Connecticut, Storrs, Connecticut 06269

[†] Institute of Materials Science, University of Connecticut,

[‡] Department of Physics, University of Connecticut,

[§] Department of Chemistry, University of Connecticut

[‡] Current address: Department of Mechanical and Aerospace Engineering, University of Virginia, Charlottesville, VA 22904-4746

* To whom correspondence should be addressed. E-mail: papadim@mail.ims.uconn.edu

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Figure S1. High resolution transmission electron micrographs of 57ECA-assisted *sem*-enriched SWNTs.

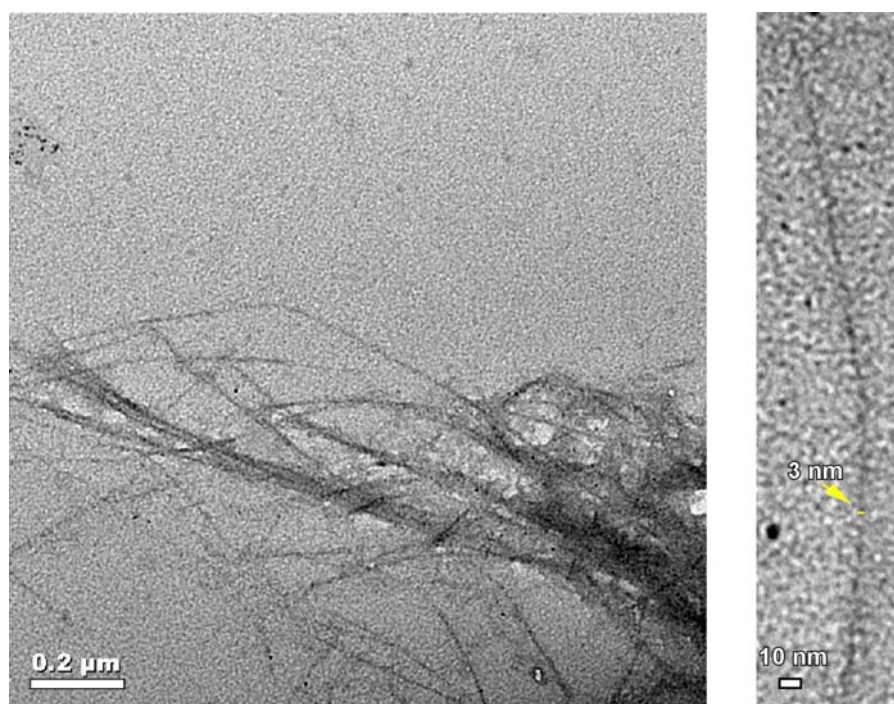


Figure S2. 2D ^1H - ^1H correlation spectroscopy (COSY) of neat 57ECA.

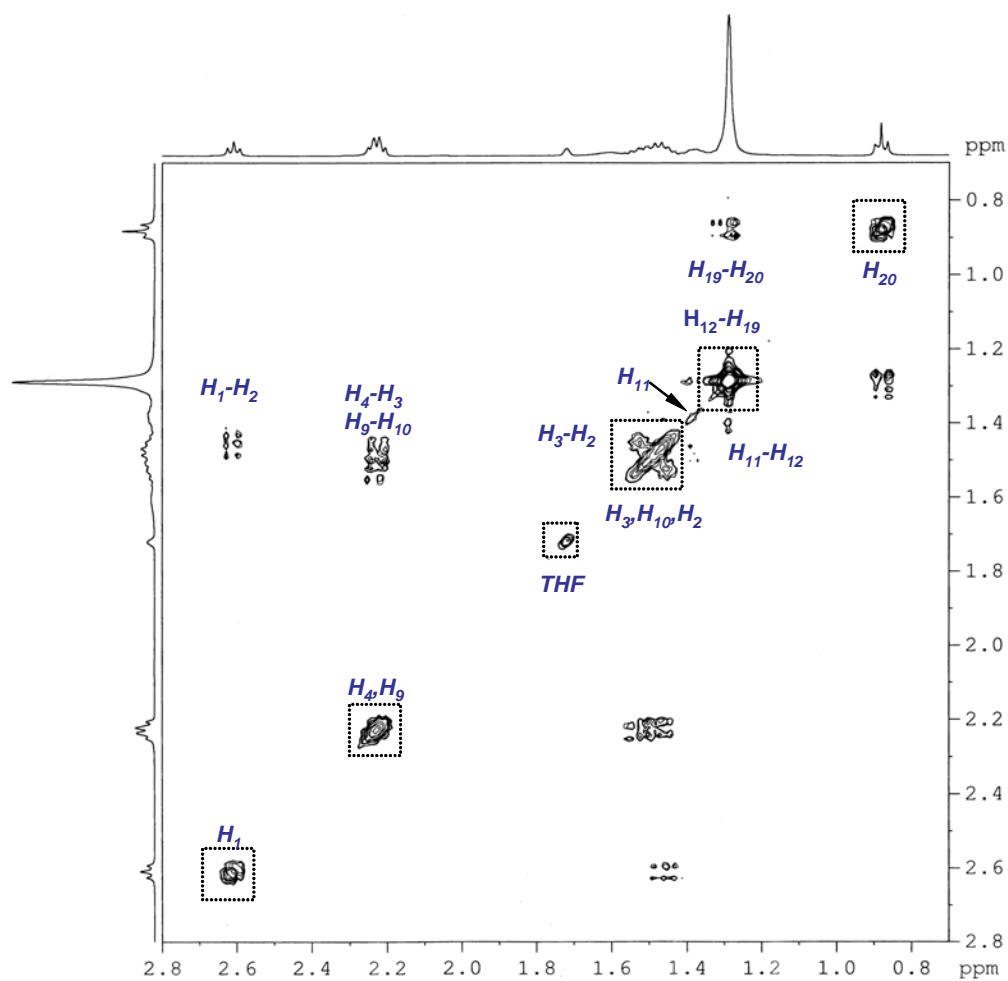


Figure S3. ^1H - ^{13}C heteronuclear multiple bond correlation (HMBC) spectra of neat 57ECA sample. Red boxes indicate direct ^1H - ^{13}C correlations (*i.e.*, $^1J_{\text{C-H}}$), while black boxes depict ^1H - ^{13}C correlations through space (*i.e.*, $^3J_{\text{C-H}}$ and $^4J_{\text{C-H}}$).

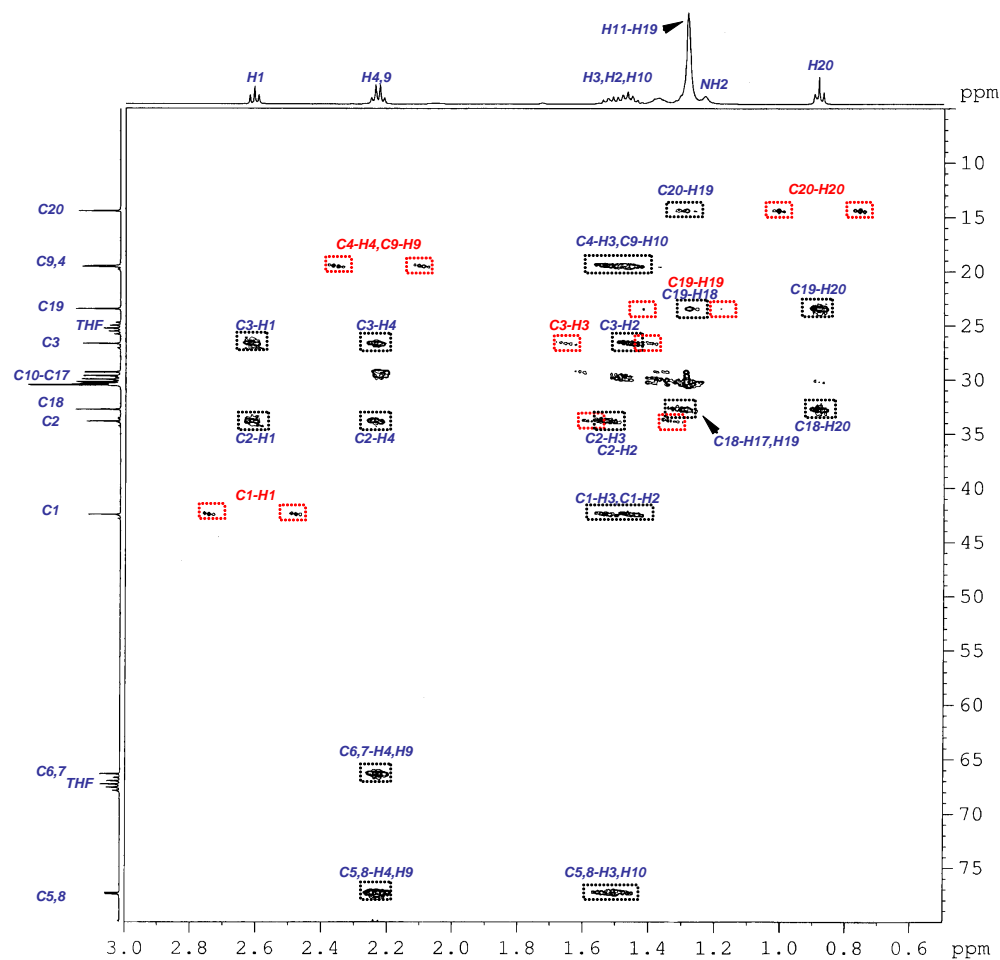


Figure S4. Close-up of the ^1H - ^{13}C heteronuclear multiple bond correlation (HMBC) spectrum of Figure S3 focusing in the C_{10} to C_{17} region.

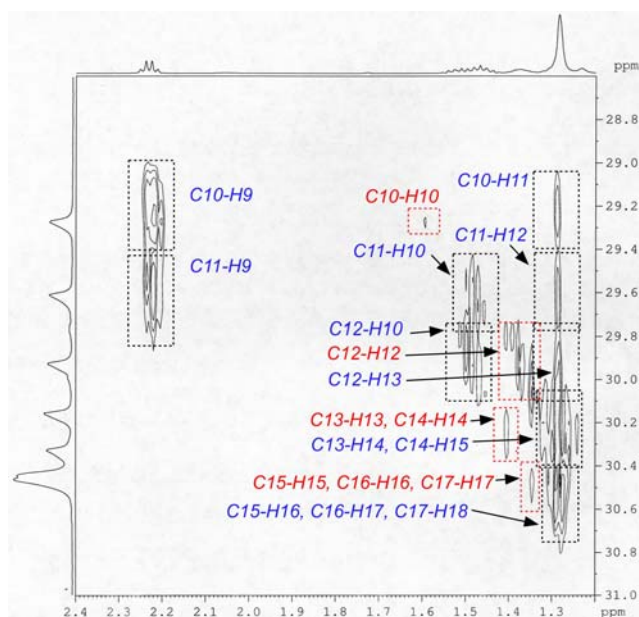


Figure S5. Effect of acidity on the 57ECA ^1H NMR position of water in THF- d_8 solution. **(A)**, **(B)**, **(C)**, and **(D)** spectra correspond to 20 μL additions of pH 5, 4, 3, and 2 HCl-acidified D_2O .

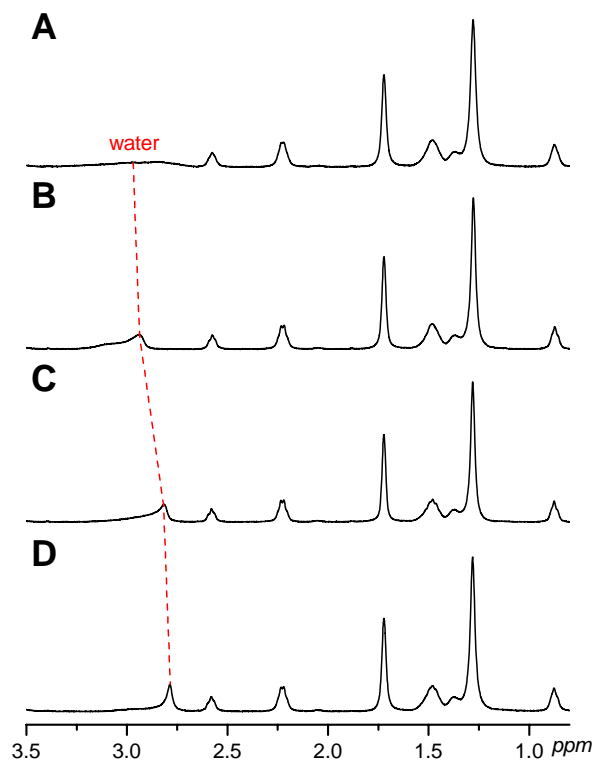


Figure S6. **(A)** ^1H NMR spectrum of ODA in THF- d_8 at 27 $^\circ\text{C}$. **(B&C)** ^1H NMR spectra of ODA-treated SWNTs at 27 and 57 $^\circ\text{C}$, respectively. This confirms that the absence of ^1H peak in **(B)**&**(C)** is not due to H_2O .

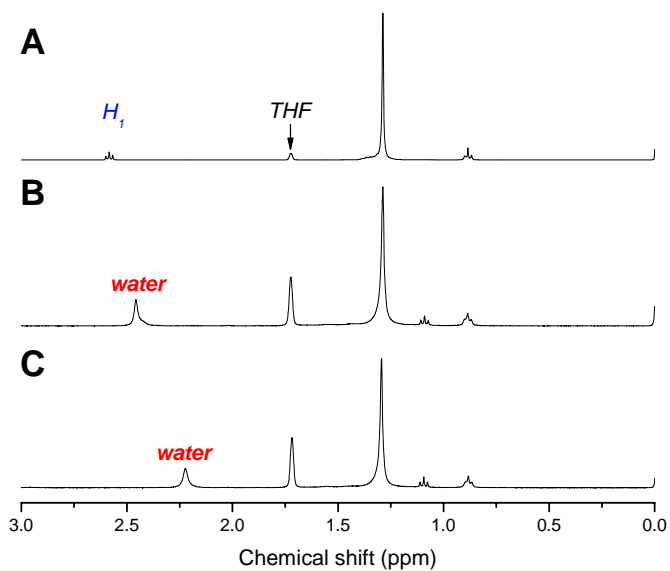
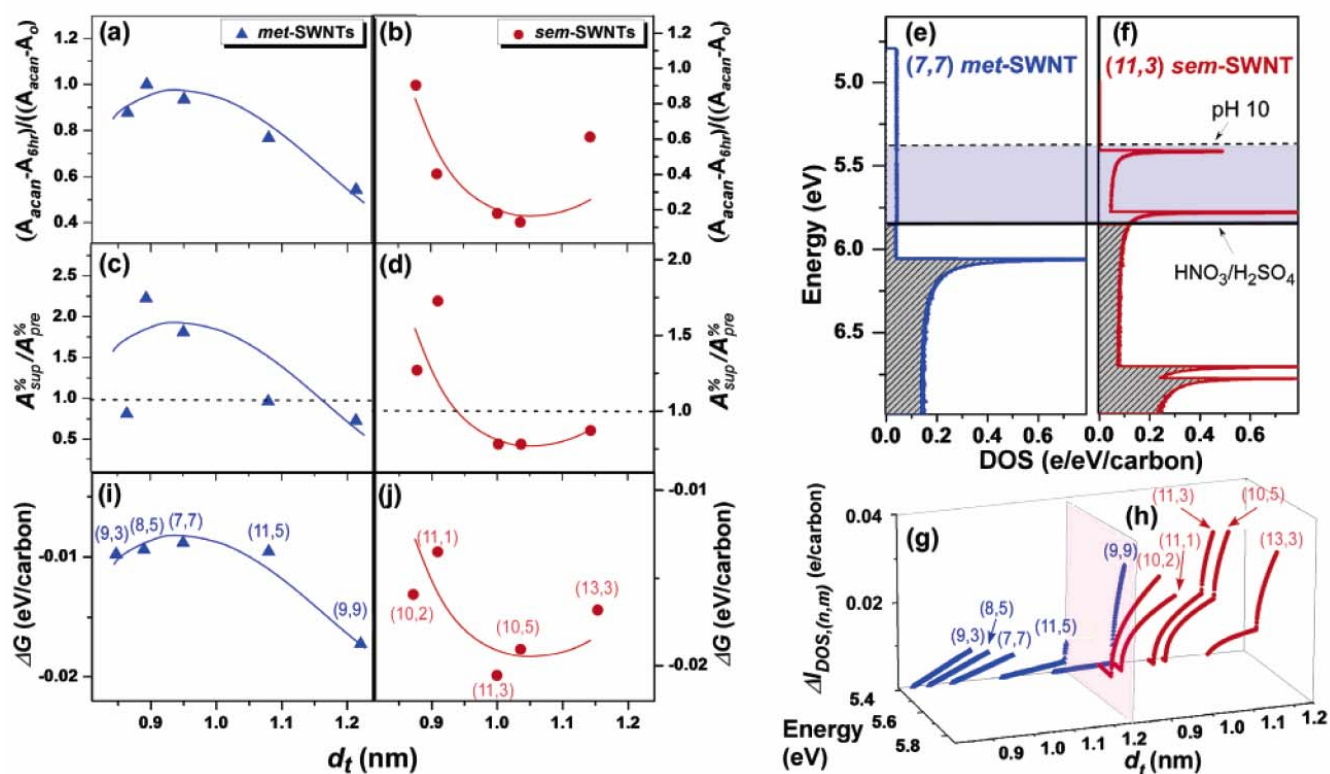


Figure S7. (a, b) Deconvoluted RRS RBM peak-area change ratios $(A_{\text{acan}} - A_{6\text{h}})/(A_{\text{acan}} - A_0)$ between annealed and 0 and 6 h DMF-aged samples as a function of diameter (d_t) for *met*- and *sem*-SWNTs. Larger $(A_{\text{acan}} - A_{6\text{h}})/(A_{\text{acan}} - A_0)$ values indicate resistance to pH of 10 assisted reduction of SWNTs toward their pristine, unoxidized state. (c, d) d_t -dependent abundance ratio in the supernatant (sup) vs precipitate (pre) fractions after 30 days of undisturbed sedimentation. Placement of the data points above or below the broken lines indicates enrichment of the respective d_t at the supernatant or precipitate, respectively. (e, f) Schematic representation of the valence density of states (DOS) with respect to vacuum for a (7,7) *met*- and (11,3) *sem*-SWNTs. The horizontal solid and broken lines racket the shaded redox jump between the estimated $\text{HNO}_3/\text{H}_2\text{SO}_4$ oxidation level and the pH 10 H^+/O_2 reduction potential, respectively. (g, h) Change of integrated DOS ($\Delta I_{\text{DOS},(n,m)}$) for representative (n,m) *met*- and *sem*-SWNTs. (i, j) Calculated reduction free energy (ΔG) for the indicated redox jump (*i.e.*, shaded region in (e&f)) as a function of d_t for *met*- and *sem*-SWNTs, respectively. The curves in parts a-d as well as i and j are for guiding the eye toward the d_t - and metallicity-dependent trends. Adapted with permission from Ref. 1, Copyright 2005 American Chemical Society.



Reference

1. Kim, S. N.; Luo, Z.; Papadimitrakopoulos, F., *Nano Lett.* 2005, 5, 2500-2504.