Supporting Information for the article entitled

"Effective Solubilization of Single-Walled Carbon Nanotubes in THF Using PEGylated Corannulene Dispersant"

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Density Functional Theory Calculations with Dispersion Corrected Functional

Accurate simulation of adsorbed species on SWNTs using DFT requires the use of empirical dispersion corrected functionals. The ωB97X-D functional used in this study has been found to provide binding energies close to MP2 benchmark calculations for polyaromatic hydrocarbons adsorbed on Boron-Nitride nanotubes.[1] This empirical dispersion correction has been applied to a number of popular functionals, providing results close to benchmark MP2 or CCSD(T) calculations.[2] Similarly, it has provided results in excellent agreement with experiment for polyaromatic hydrocarbons adsorbed on graphene with 6-31G* basis set.[3]

SWNTs were constructed using C-C bond lengths of 1.421Å. Geometry optimization of the adsorbed species on SWNTs was carried out at the ωB97X-D/6-31G* level of theory while nanotube coordinates held fixed. The binding energy was calculated according to

$$U_b = E_A + E_{CNT} - E_{A\text{-}CNT} \tag{1}$$

where U_b is the binding energy, E_A is the total energy of adsorbate optimized at the ωB97X-D/6-31G* level of theory, E_{CNT} is the total energy of the SWNT from a single-point calculation, and $E_{A\text{-}CNT}$ is the total energy of the optimized SWNT-adsorbate complex. Counterpoise correction was applied to account for basis set superposition error (BSSE).

1.   Y. Zhao, X. Wu, J. Yang and X. Cheng Zeng, *Physical Chemistry Chemical Physics*, 2011, **13**, 11766-11772.
2.   S. Grimme, *Journal of computational chemistry*, 2006, **27**, 1787-1799.
3.   O. V. Ershova, T. C. Lillestolen and E. Bichoutskaia, *Physical Chemistry Chemical Physics*, 2010, **12**, 6483-6491.
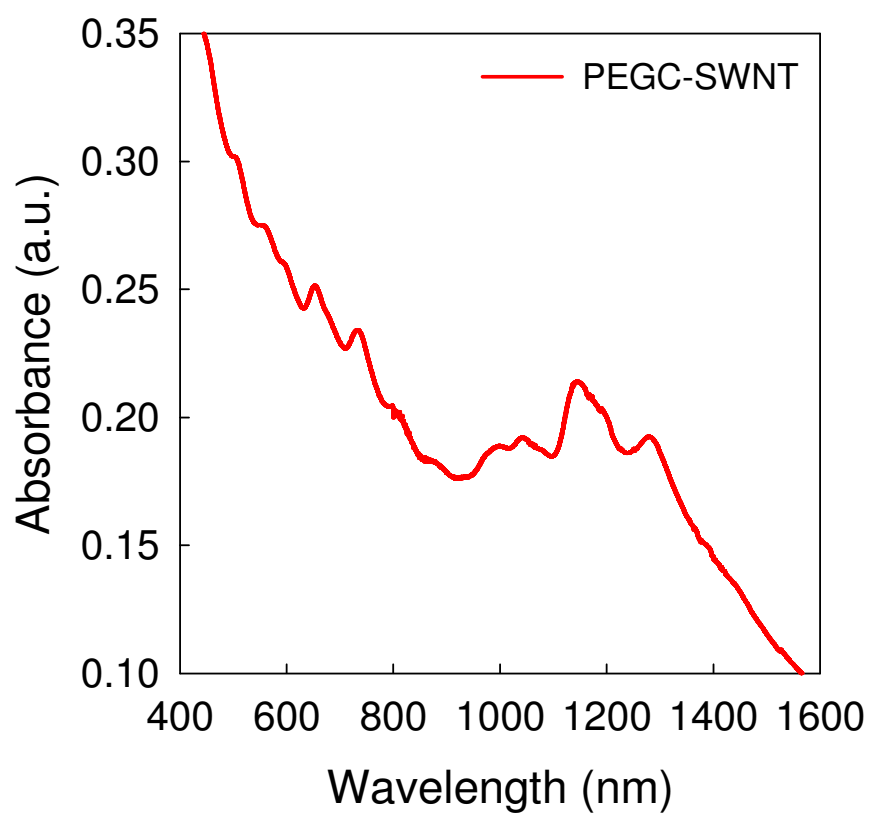
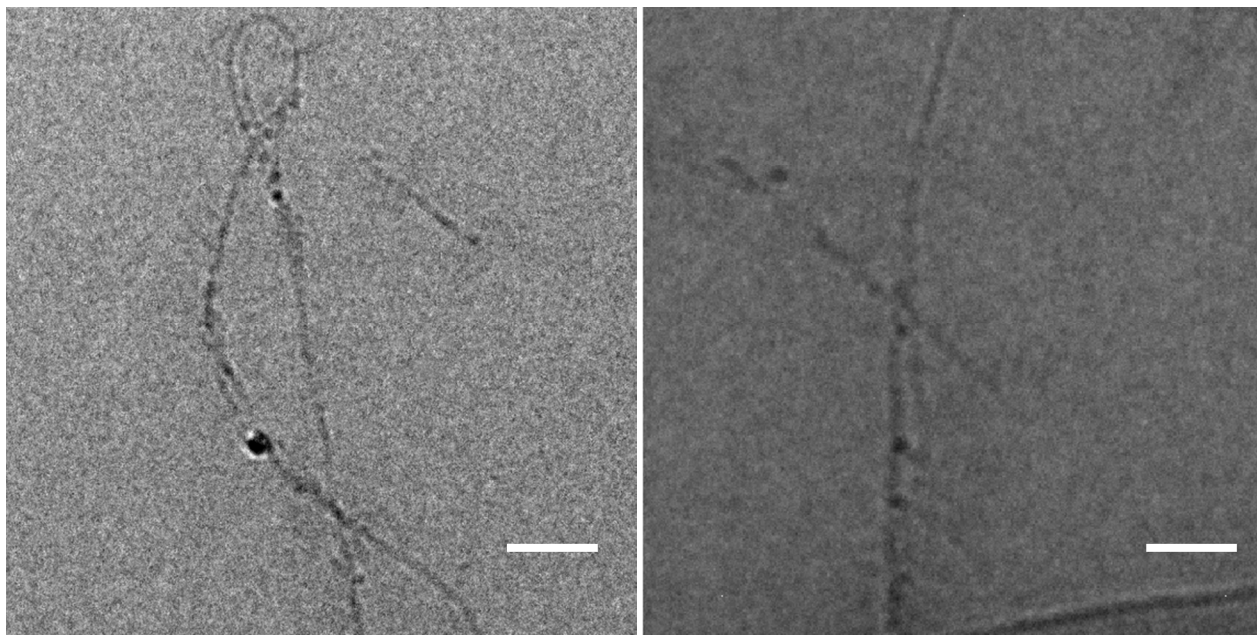**Figure S1.** PEGC-SWNT absorption between 400 and 1600 nm.

Figure S2. Sample transmission electron microscope (TEM) images prepared from dilute solution of PEGC-SWNT sample. Some circular features are present on nanotube surfaces. These features can be attributed to adsorbed PEGC molecules. Dark spots could be a result of aggregation of PEGC on SWNT surface upon drying during sample preparation. TEM images were collected with JEOL JEM-100 CX II transmission electron microscope. The scale bar corresponds to 100 nm.

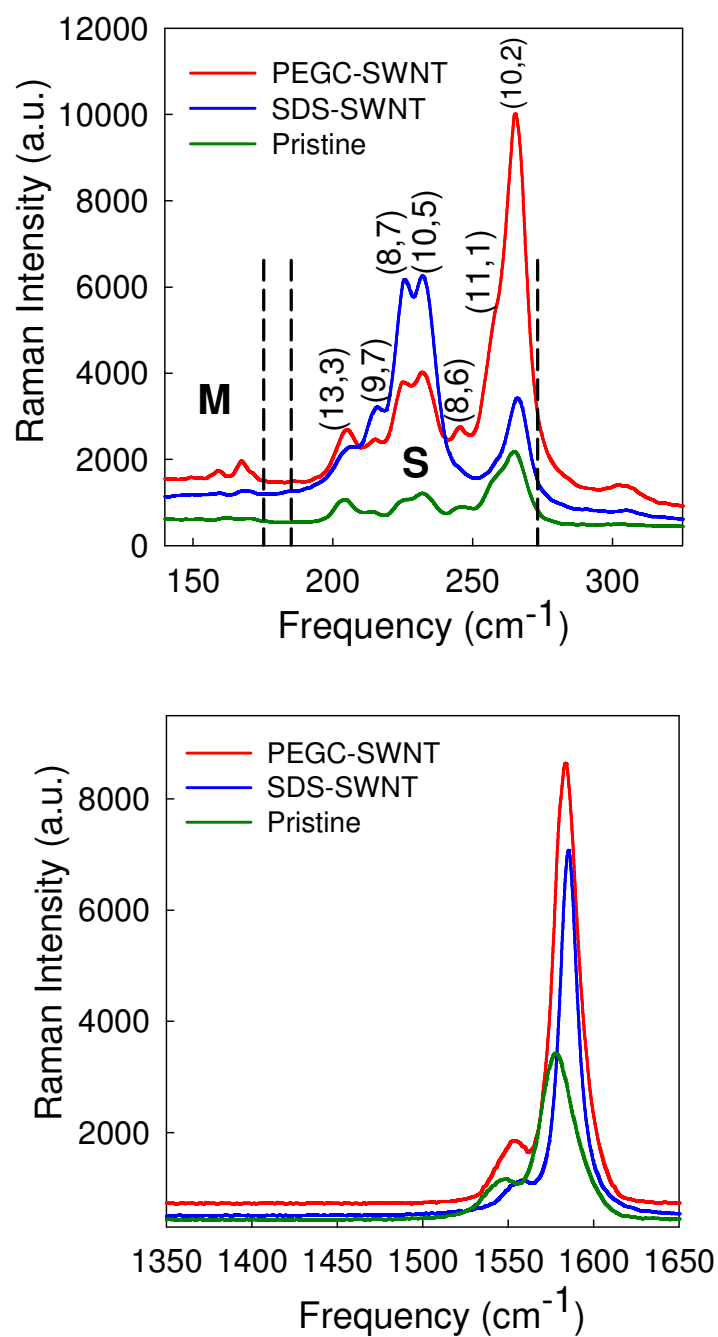**Figure S3.** Raman spectra obtained for PEGC-SWNT, SDS-SWNT, and pristine samples with a 785 nm excitation laser line.