

Supplemental Materials:

**Morphology and Stability of Polycarbazole Wrapped
Carbon Nanotubes: Joint Experimental and
Computational Studies**

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We have generated the initial structures of single walled carbon nanotubes (SWNT) wrapped by oligocarbazole isomers with the 2-ethylhexyl side chains attached to the pyrrole rings at the ‘same side’ and at the ‘opposed-side’ of each neighboring unit with a reference to the main carbazole backbone. Then these initial structures are optimized using MM3 force field, as describe in the main text of the paper. The binding energies between the SWNT and the hexamer of carbazole of the optimized hybrids are compared in Figure S1 to determine the effect of the initial alignment of side groups. In the isolated pristine carbazole polymers the structures with the side groups on the alternating sides is the most energetically preferable due to a strong steric repulsion between the side chains. Geometry optimization of oligocarbazole-SWNTs hybrids allows for ample opportunities for the side chains to switch sides resulted in final structures that are almost independent on their initial configurations. Overall, in the optimized structures of hybrids, both 2,7- and 3,6-isomers demonstrate pretty random twisting behavior of side chains, with their more frequent alignments at the alternating sides. Therefore, the binding energy between the nanotube and the oligocarbazole started from the ‘same side’ or the ‘opposed-side’ is comparable, showing an energy difference of an order of thermal fluctuations. However, there are a few configurations, where the system is trapped in a local minima, when it is started either from the same or the alternating sides. Any dependence for either 2,7- or 3,6-oligocarbazole on initial wrapping geometry appears to be too subtle to play a predominant role in influencing some specific trends in the final structure after geometry optimization, making the relationship between the initial and final structures somewhat arbitrary. As such, our approach of probing numerous initial wrapping conformation seems reasonable in finding the most probable hybrid morphology.

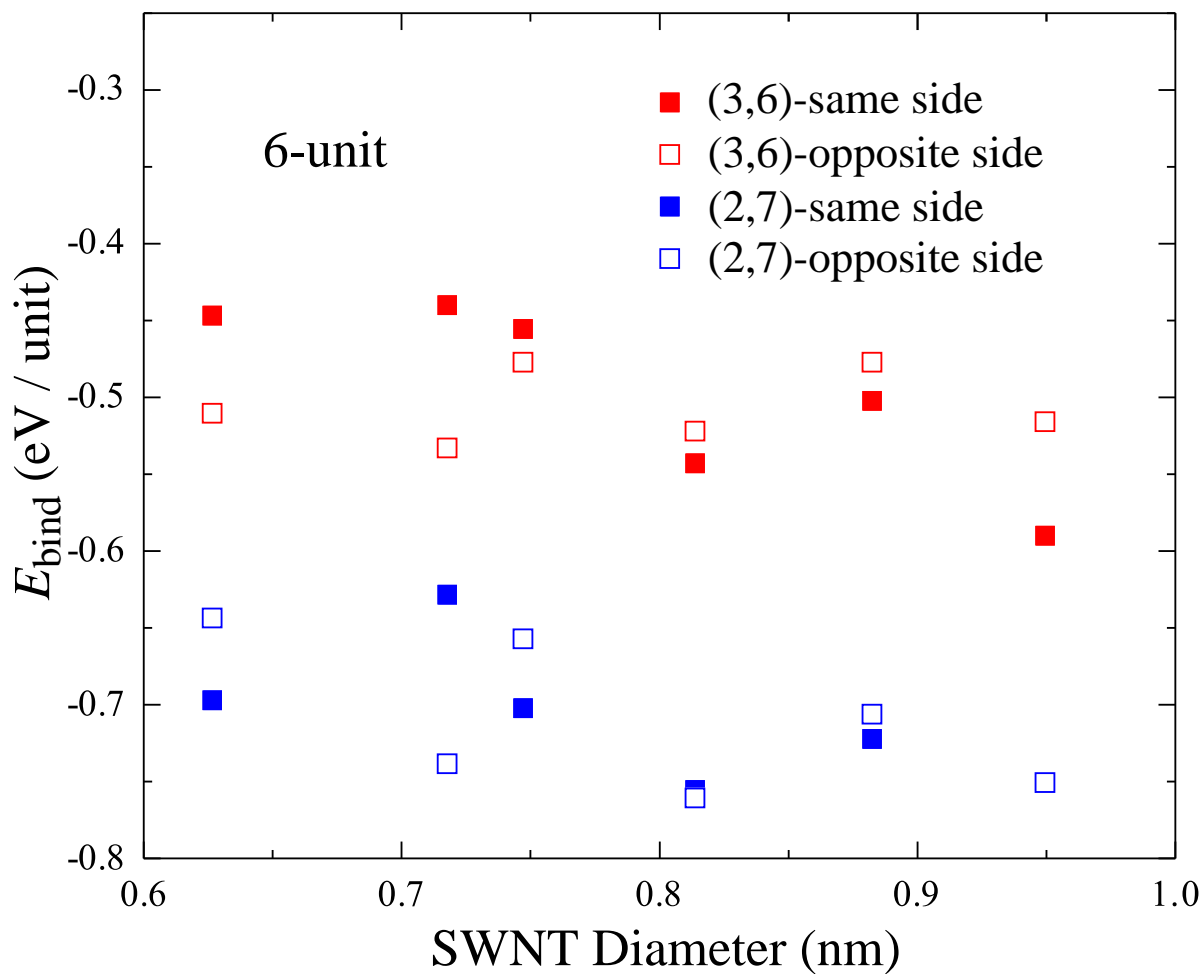


Figure 1: **S1**: Binding energy vs. nanotube diameter for SWNTs wrapped in oligocarbazole isomers of 6 units in length with initial alignment of the 2-ethylhexyl side chains attached to the pyrrole rings at the 'same side' and at the 'opposed-side' of each neighboring unit.

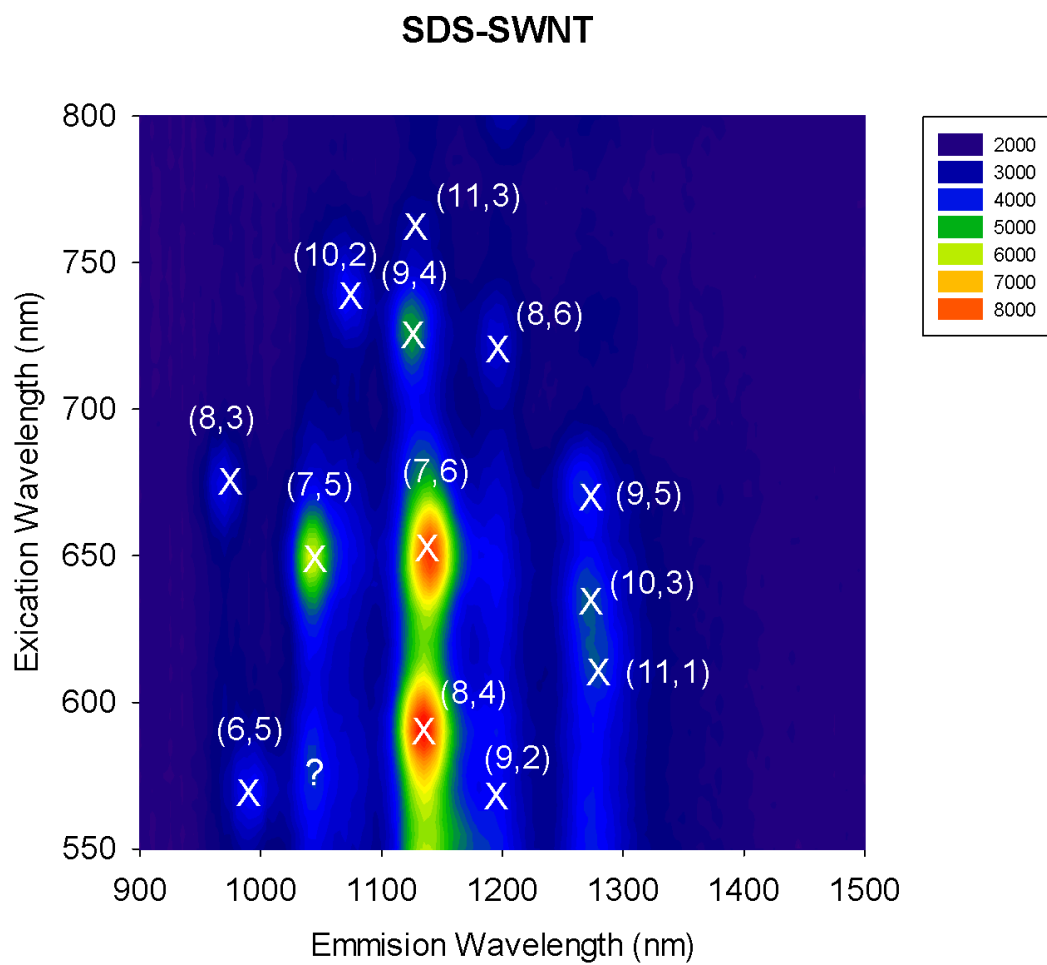


Figure 2: **S2:** PL contour map of HiPco SWNTs dispersed in SDS in D₂O

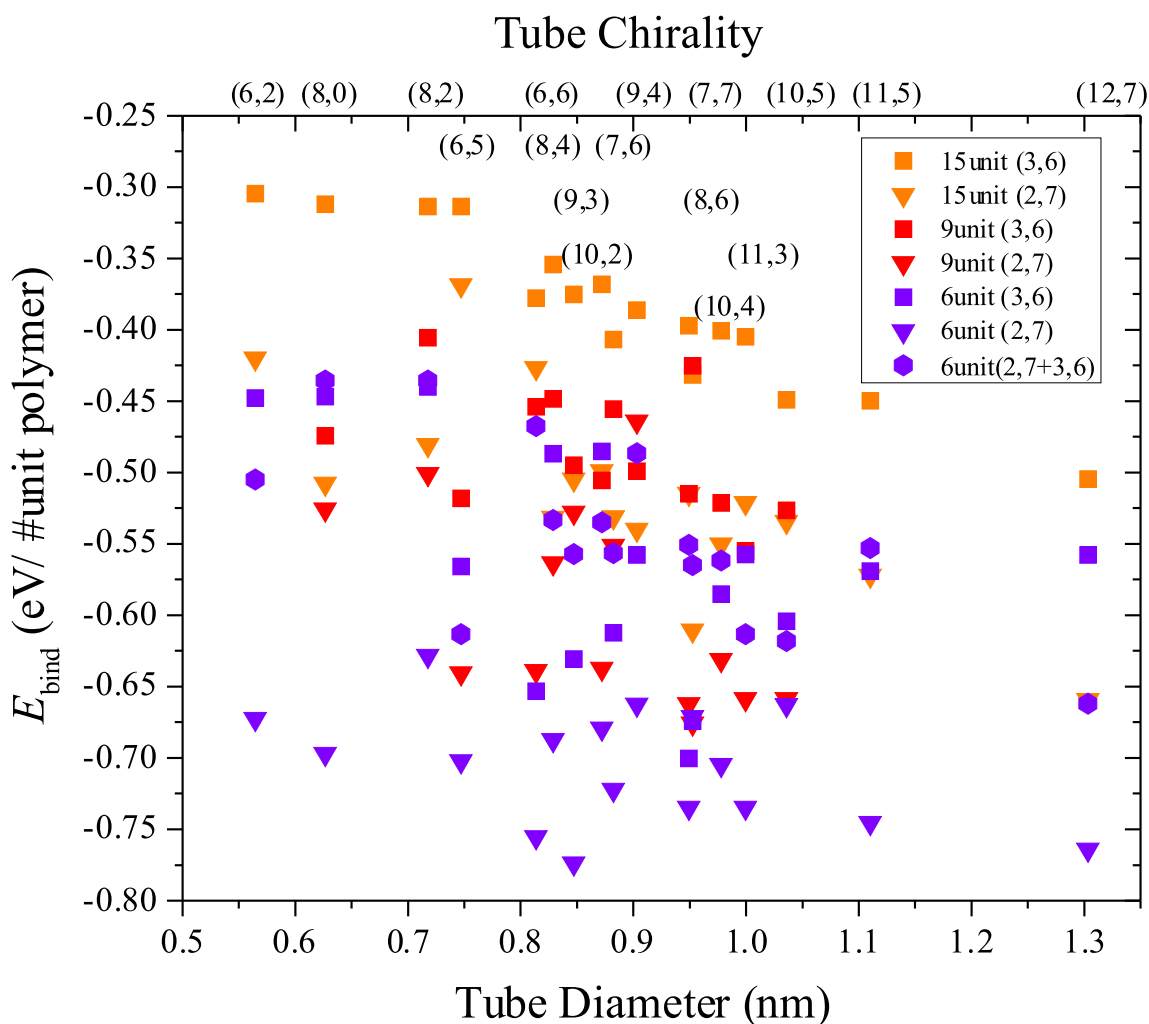


Figure 3: **S3**: The binding energy between the SWNTs and 2,7-, 3,6-, and 2,7-3,6-isomers of oligocarbazoles of various length (15, 9, and 6 units) as a function of the nanotube diameter and chirality. The binding energy decreases with the oligocarbazole length. The 2,7-isomers provide the most stable oligocarbazole-SWNT hybrids, while 3,6- and 2,7-3,6 isomers have comparable interaction strengths with the nanotubes. Chirality selectivity in the binding energy is strongly effected by the length and type of oligocarbazole. For long chains of 15 and 9 units in length, all isomers have the least binding with the (8,2) nanotube. Considering the SWNTs with diameters ≤ 1 , most of isomers have the strongest or the second strongest interaction with the (8,6) SWNT. However, binding with the (6,5) is very strong for 3,6- and 2,7-3,6-isomers of 6 and 9 units in length, but is the weakest for those isomers of 15-units in length.