Supporting Information for

Revealing the Tunability of Electronic Structures and Optical Properties of Novel SWCNT Derivatives, Phenine Nanotubes

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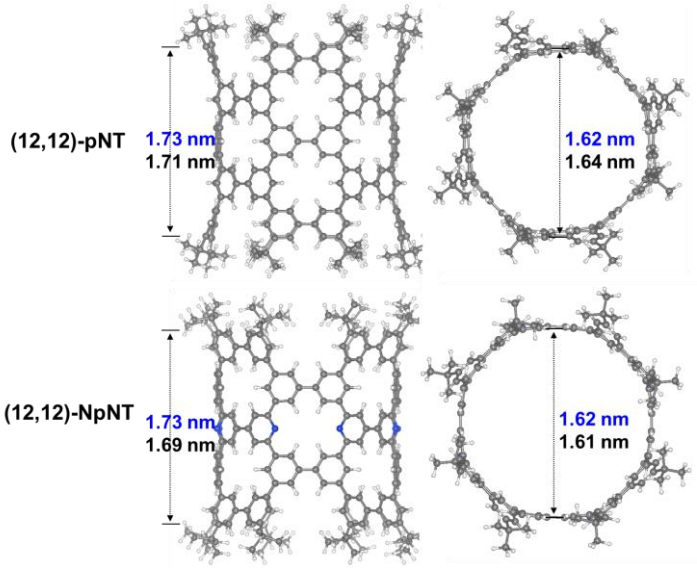

Figure S1. Experimental and theoretical results for the length and diameter of (12,12)-pNT and (12,12)-NpNT. The values in blue show our theoretical results, while the black ones show the experimental data.

Table S1. Details of the HOMO-LUMO energy levels and the gaps of (12,12)-pNT and 1212pNT, together with their lowest excitation energy and corresponding oscillator strength (*f*).

Structure	**HOMO**	**LUMO**	**H-L gap** (eV)	S_0-S_1(nm)	***f***
(12,12)-pNT	-3.371	0.327	3.698	335	0.0000
1212pNT	-3.559	0.179	3.738	331	0.0000

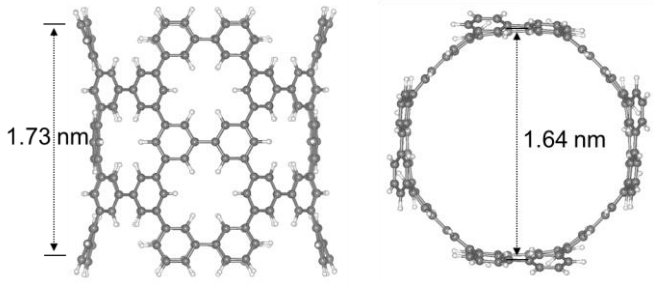

Figure S2. Theoretically predicted structural parameters of 1212pNT with edge sp^2-carbons terminated by hydrogen atoms.

Table S2. Oscillator strengths of the lowest 10 vertical excitations of all the studied structures.

Transitions	Pre-99pNT	99pNT	99pNT-L1	99pNT-L2	99pNT-L3	1212pNT	1515pNT
$S_0 \rightarrow S_1$	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$S_0 \rightarrow S_2$	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$S_0 \rightarrow S_3$	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$S_0 \rightarrow S_4$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$S_0 \rightarrow S_5$	0.0008	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$S_0 \rightarrow S_6$	0.0008	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$S_0 \rightarrow S_7$	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$S_0 \rightarrow S_8$	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
$S_0 \rightarrow S_9$	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
$S_0 \rightarrow S_{10}$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Transitions	1818pNT	99pNT-2N	99pNT-4N	99pNT-6N	99pNT-L3-6N	99pNT-2H	99pNT-4H
$S_0 \rightarrow S_1$	0.0000	0.0000	0.0000	0.0000	0.0000	0.3662	0.0012
$S_0 \rightarrow S_2$	0.0000	0.0001	0.0000	0.0000	0.0000	0.0017	0.0008
$S_0 \rightarrow S_3$	0.0000	0.0017	0.0010	0.0000	0.0000	0.0022	0.2826
$S_0 \rightarrow S_4$	0.0000	0.0017	0.0001	0.0000	0.0000	0.1451	0.0966
$S_0 \rightarrow S_5$	0.0000	0.0002	0.0009	0.0000	0.0000	0.0203	0.1187
$S_0 \rightarrow S_6$	0.0000	0.0000	0.0022	0.0000	0.0000	0.0010	0.0011
$S_0 \rightarrow S_7$	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0033
$S_0 \rightarrow S_8$	0.0000	0.0069	0.0033	0.0002	0.0000	0.0017	0.4857
$S_0 \rightarrow S_9$	0.0001	0.0001	0.0008	0.0000	0.0000	0.0027	0.0236
$S_0 \rightarrow S_{10}$	0.0001	0.0007	0.0000	0.0000	0.0000	0.1083	0.0003

Transitions	99pNT-6H	99pNT-L3-2H	1212pNT-2H	1212pNT-4H	1212pNT-8H
$S_0 \rightarrow S_1$	0.0008	0.3223	0.6810	0.0019	0.0000
$S_0 \rightarrow S_2$	0.0017	0.0003	0.0002	0.0014	0.0003
$S_0 \rightarrow S_3$	0.0005	0.0017	0.0006	0.7870	0.0003
$S_0 \rightarrow S_4$	0.0002	0.0001	0.0931	0.0148	0.0000
$S_0 \rightarrow S_5$	0.0012	0.0007	0.0000	0.3373	0.0000
$S_0 \rightarrow S_6$	0.0000	0.0000	0.0009	0.0000	0.0043
$S_0 \rightarrow S_7$	0.0001	0.0002	0.0005	0.0311	0.0043
$S_0 \rightarrow S_8$	0.7859	0.0001	0.0178	0.0006	0.0000
$S_0 \rightarrow S_9$	0.0005	0.0331	0.0004	0.3610	0.0000
$S_0 \rightarrow S_{10}$	0.7012	0.0008	0.0101	0.0125	0.0004

Table S3. Ground state HOMO-LUMO energy levels and corresponding gaps of the studied phenine nanotubes (energy unit in eV).

	Pre-99pNT	**99pNT**	**99pNT-L1**	**99pNT-L2**	**99pNT-L3**	**1212pNT**	**1515pNT**
LUMO	0.306	0.185	0.115	0.077	0.044	0.179	0.168
HOMO	-3.535	-3.554	-3.593	-3.615	-3.627	-3.559	-3.563
H-L gap	3.841	3.739	3.708	3.693	3.671	3.738	3.731
	1818pNT	**99pNT-2N**	**99pNT-4N**	**99pNT-6N**	**99pNT-L3-6N**	**99pNT-2H**	**99pNT-4H**
LUMO	0.158	-0.514	-0.515	-0.511	-0.635	-0.566	-0.589
HOMO	-3.568	-3.561	-3.578	-3.626	-3.637	-2.356	-2.354
H-L gap	3.726	3.046	3.063	3.116	3.001	1.790	1.765
	99pNT-6H	**99pNT-L3-2H**	**1212pNT-2H**	**1212pNT-4H**	**1212pNT-8H**		
LUMO	-0.594	-0.689	-0.644	-0.655	-0.667		
HOMO	-2.353	-2.484	-2.391	-2.381	-2.372		
H-L gap	1.759	1.795	1.747	1.726	1.705		

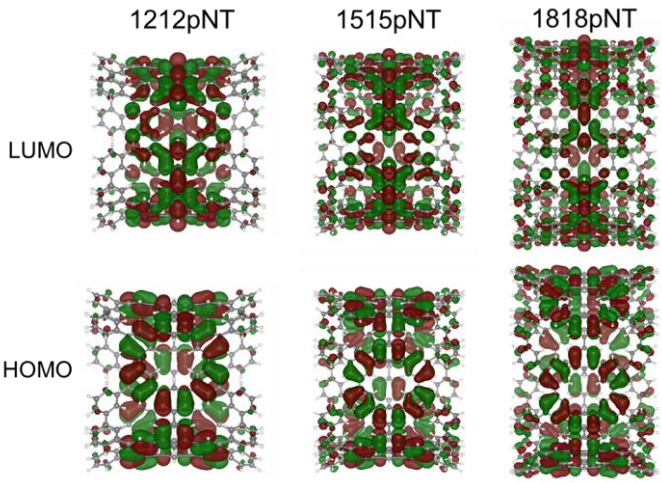

Figure S3. Ground-state HOMO and LUMO spatial distributions of phenine nanotubes with varying diameters.