Electronic Supplementary Information

"Effects of chirality and diameter of single-walled carbon nanotubes on their structural stability and solubility parameters"

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Computational Methods

All calculations were done with the Materials Studio modeling software platform (ver. 6.0, Accelrys, San Diego, USA) with the COMPASS (condensed phase optimized molecular potentials for atomistic simulation studies) forcefield. We also followed the protocol established in our earlier study for the modeling of SWCNTs with finite-length model and the calculation of the solubility parameters. For calculations of the structural stability of SWCNTs, NPT dynamics was applied to 3 sets of armchair and zigzag SWCNTs, the diameters and lengths of which were nearly identical: (6,6) and (10,0), (7,7) and (12,0), and (8,8) and (14,0). The applied pressure ranged from 0.05 to 2 GPa.

Table S1. Determined solubility parameters of armchair and zigzag SWCNTs with variation of the diameter

SWCNT		Diameter [nm]	Density [g/cm^3]	δ [(J/cm^3)$^{1/2}$]	δ_{vdW} [(J/cm^3)$^{1/2}$]	δ_{es} [(J/cm^3)$^{1/2}$]
Armchair	(3,3)	0.41	1.50	20.76	20.81	0
	(4,4)	0.54	1.50	19.66	19.69	0
	(5,5)	0.68	1.45	18.49	18.47	0.72
	(6,6)	0.81	1.43	18.32	18.33	0.24
	(7,7)	0.95	1.43	18.49	18.47	0.85
	(8,8)	1.09	1.43	18.60	18.58	0.87
	(9,9)	1.22	1.46	18.90	18.87	0.99
	(10,10)	1.36	1.44	19.07	19.10	0
	(11,11)	1.49	1.46	18.99	18.98	0.62
Zigzag	(6,0)	0.47	1.52	19.70	19.70	0.18
	(7,0)	0.55	1.48	18.93	18.93	0
	(8,0)	0.63	1.48	18.84	18.89	0
	(9,0)	0.70	1.46	18.47	18.50	0
	(10,0)	0.78	1.43	17.84	17.87	0
	(11,0)	0.86	1.39	17.42	17.41	0.65
	(12,0)	0.94	1.33	16.56	16.56	0.15
	(13,0)	1.02	1.29	16.40	16.41	0
	(14,0)	1.10	1.33	16.86	16.86	0.07
	(15,0)	1.17	1.32	16.95	16.93	0.65
	(16,0)	1.25	1.31	17.06	17.06	0.39
	(17,0)	1.33	1.32	17.19	17.21	0
	(18,0)	1.41	1.31	17.56	17.62	0
	(19,0)	1.49	1.38	18.06	18.10	0

Table S2. Comparison of structural and chemical parameters of SWCNTS as shown in the Figure 3

CNT	Diameter [nm]	Length [nm]	Chemical Formula	Molar mass [g/mol]
(8,8) SWCNT	1.09	3.44	$C_{448}H_{32}$	5413.18
(14,0) SWCNT	1.10	3.55	$C_{448}H_{28}$	5409.15

Table S3. Effects of the diameter and chirality of SWCNTs on the mechanical parameters reported in the literature.

Parameters	Chirality	Diameter
Collapse pressure	Independent	Inverse proportionality
Bending rigidity	A < Z	Not studied
Torsional buckling	A < Z	Not studied
Shear modulus	A < Z but not significant	Dependent (< 2nm) Independent (> 2nm)
Young's modulus	Independent	Independent
Compressive force	A < Z (< 10nm) Independent (> 10nm)	Inverse proportionality

* A: armchair, Z: zigzag

Table S4. Eccentricities of various SWCNTs with varying the applied pressure

Pressure [GPa]	**0.05**	**0.1**	**0.2**	**0.3**	**0.5**	**1.0**	**2.0**
(6,6) SWCNT	0.369	0.476	0.488	0.613	0.507	0.711	0.771
(10,0) SWCNT	0.147	0.425	0.441	0.348	0.323	0.556	0.553
(7,7) SWCNT	0.758	0.769	0.746	0.738	0.743	0.829	0.695*
(12,0) SWCNT	0.504	0.511	0.512	0.559	0.569	0.819	0.873
(8,8) SWCNT	0.806	0.820	0.853	0.833	0.837*	0.729*	0.603*
(14,0) SWCNT	0.462	0.746	0.774	0.742	0.795	0.768*	0.847*

* For certain higher applied pressure, the NPT dynamics failed to complete full dynamics steps, because the energy deviation exceeds the maximum value due to the collapse of SWCNT structure.