

Electronic Supplementary Information

“Determination of solubility parameters of single-walled and double-walled carbon nanotubes using a finite-length model”

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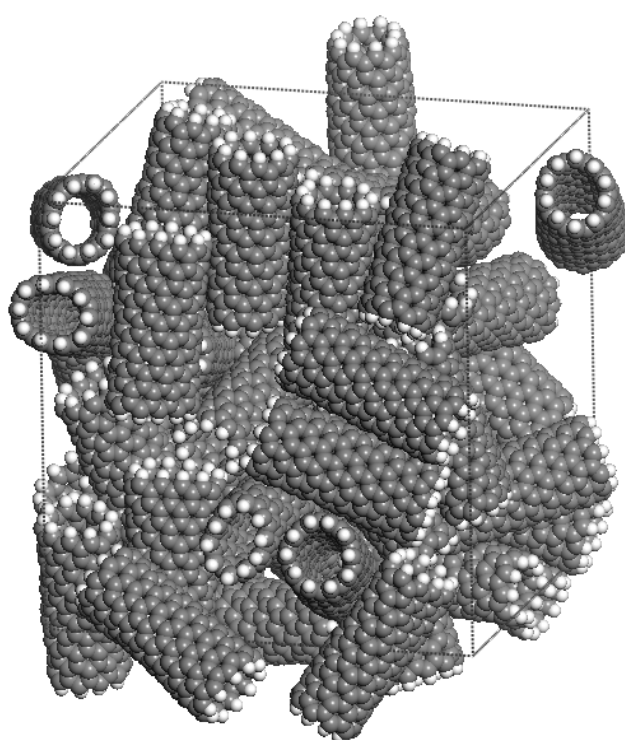


Figure S1. Configuration of the cell containing fifty (10,0) SWCNTs.

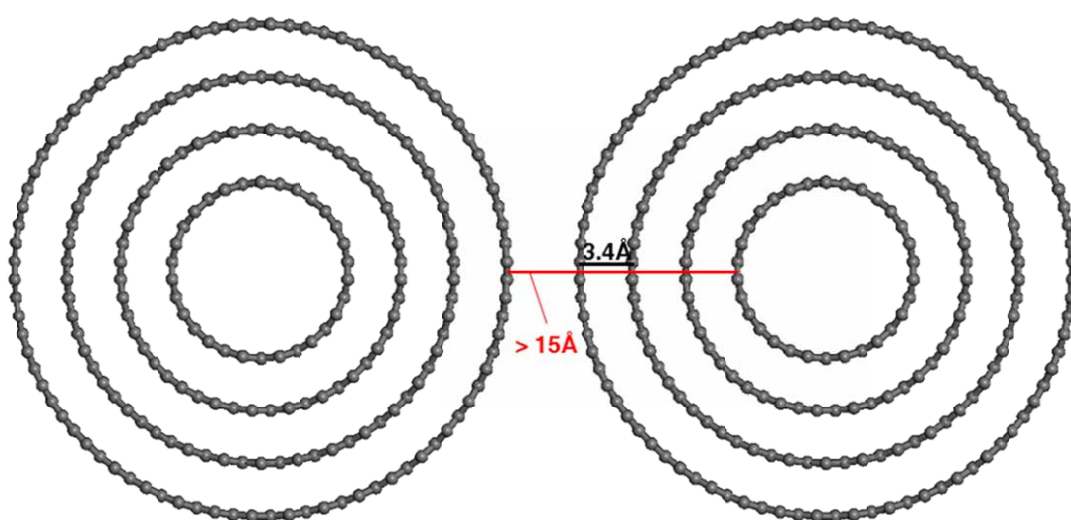


Figure S2. The distance between an atom of outer-most (first) wall in a MWCNT and an atom of fourth wall in another MWCNT.

Table S1. Determined solubility parameters for (6,6) and (10,0) SWCNTs as a function of the length

CNT	Diameter [nm]	Length [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}]
(6,6) SWCNT-1	0.81	0.24	0.96	19.54	19.29	3.15
(6,6) SWCNT-2	0.81	0.49	1.15	18.66	18.23	4.00
(6,6) SWCNT-3	0.81	0.74	1.27	18.63	18.46	2.47
(6,6) SWCNT-4	0.81	0.98	1.34	18.76	18.72	1.33
(6,6) SWCNT-5	0.81	1.23	1.40	18.93	18.88	1.47
(6,6) SWCNT-6	0.81	1.48	1.43	18.99	18.97	1.09
(6,6) SWCNT-7	0.81	1.72	1.44	18.76	18.72	1.22
(6,6) SWCNT-8	0.81	1.97	1.45	18.69	18.68	0.54
(6,6) SWCNT-9	0.81	2.21	1.45	18.46	18.50	0
(6,6) SWCNT-10	0.81	2.46	1.45	18.31	18.30	0.74
(6,6) SWCNT-11	0.81	2.70	1.46	18.28	18.26	0.80
(6,6) SWCNT-12	0.81	2.95	1.44	17.90	17.88	0.88
(10,0) SWCNT-1	0.78	0.43	1.10	17.73	17.33	3.71
(10,0) SWCNT-2	0.78	0.85	1.27	17.80	17.72	1.67
(10,0) SWCNT-3	0.78	1.28	1.38	18.36	18.38	0
(10,0) SWCNT-4	0.78	1.70	1.44	18.52	18.54	0
(10,0) SWCNT-5	0.78	2.13	1.43	18.07	18.13	0
(10,0) SWCNT-6	0.78	2.56	1.42	17.58	17.56	0.82
(10,0) SWCNT-7	0.78	2.98	1.41	17.14	17.14	0.43

Table S2. Determined solubility parameters for SWCNTs and DWCNTs as a function of the diameter

CNT	Diameter [nm]	Length [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}]
(6,0) SWCNT-5	0.47	2.13	1.52	19.70	19.70	0.18
(10,0) SWCNT-5	0.78	2.13	1.43	18.07	18.13	0
(15,0) SWCNT-5	1.17	2.13	1.32	16.95	16.93	0.65
(6,0)(15,0) DWCNT-5	1.17	2.13	1.49	22.77	22.88	0
(15,0)(24,0) DWCNT-5	1.88	2.13	1.43	22.63	22.79	0
(24,0)(33,0) DWCNT-5	2.58	2.13	1.40	21.96	22.08	0