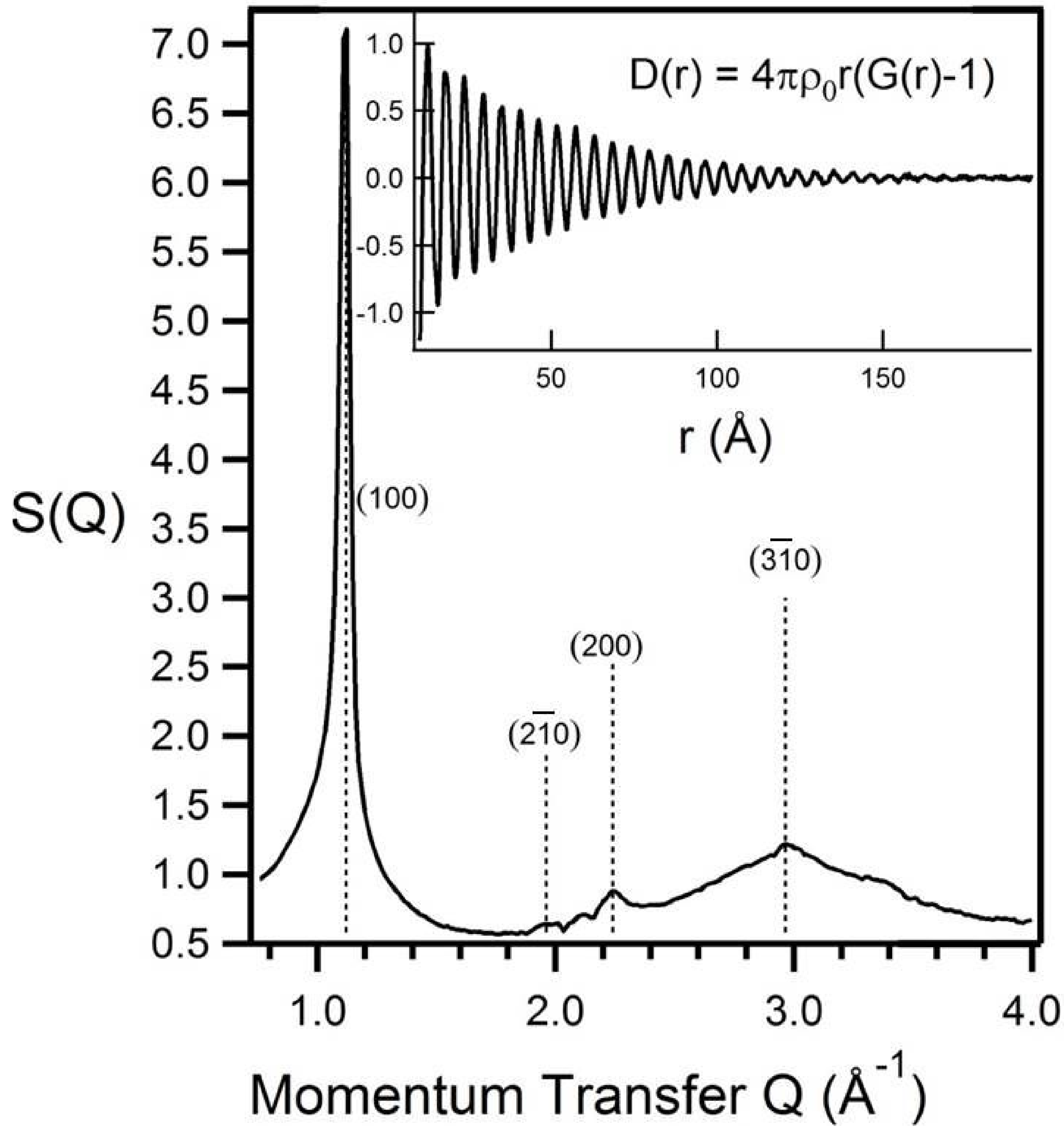
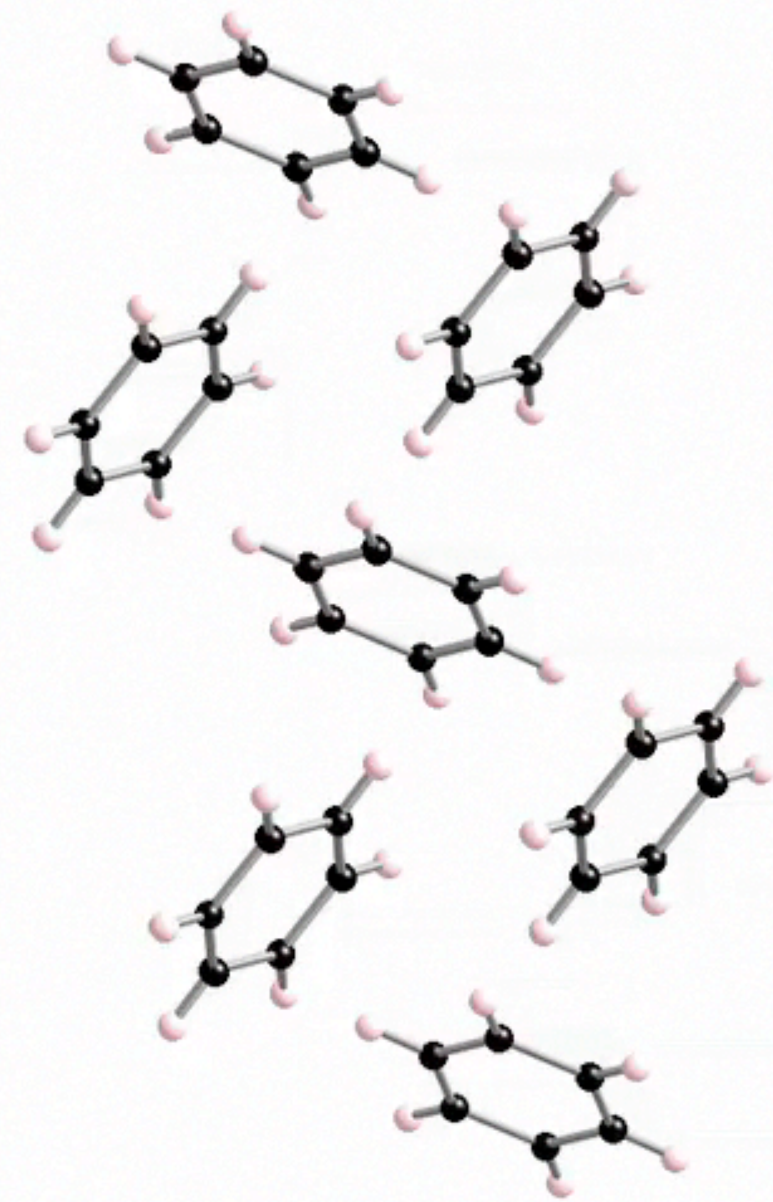
Nanothreads

Compress benzene in a diamond anvil cell…





Smallest Nanotube: Breaking the Symmetry of sp^3 Bonds in Tubular Geometries

Dragan Stojkovic, Peihong Zhang, and Vincent H. Crespi*

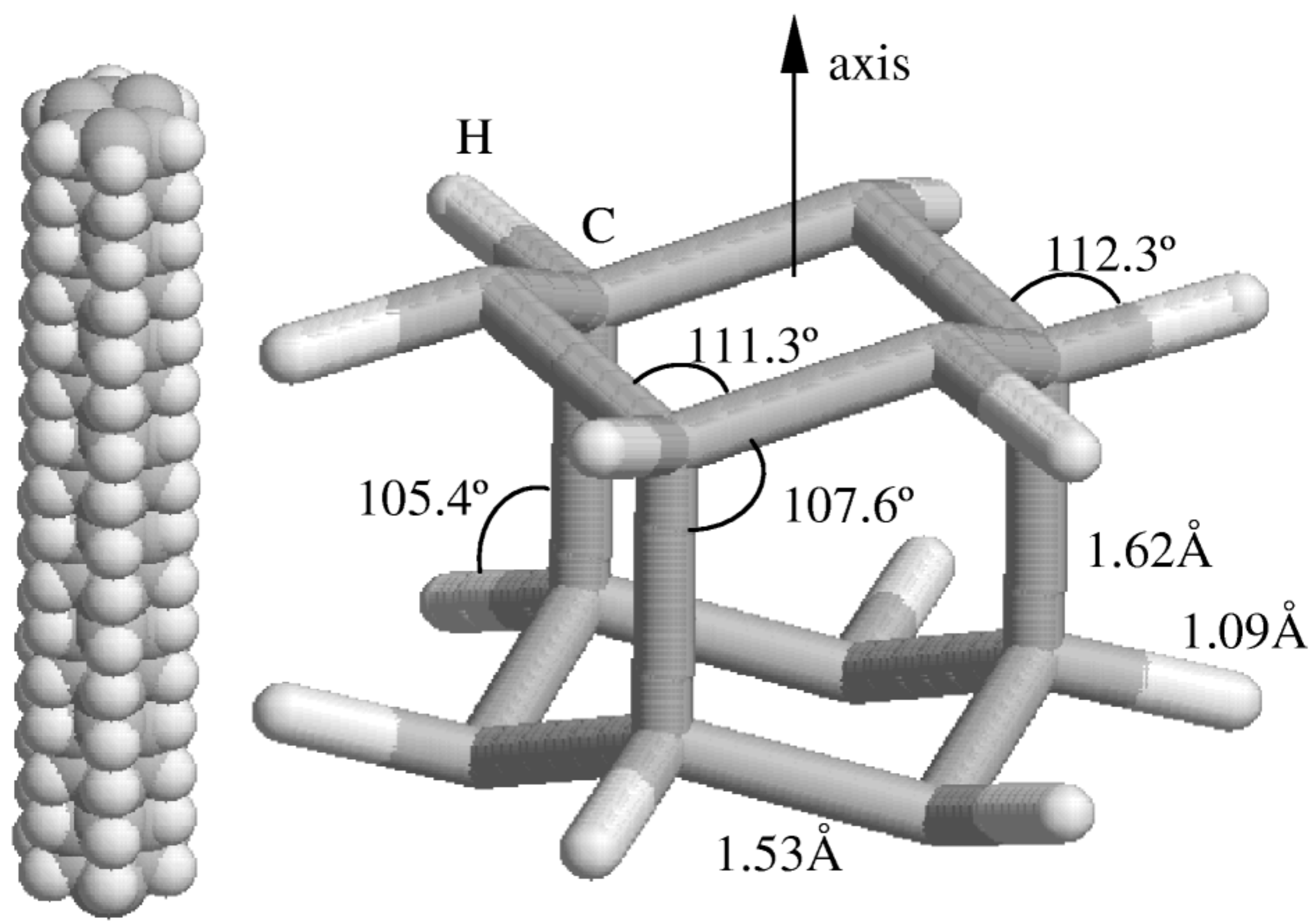
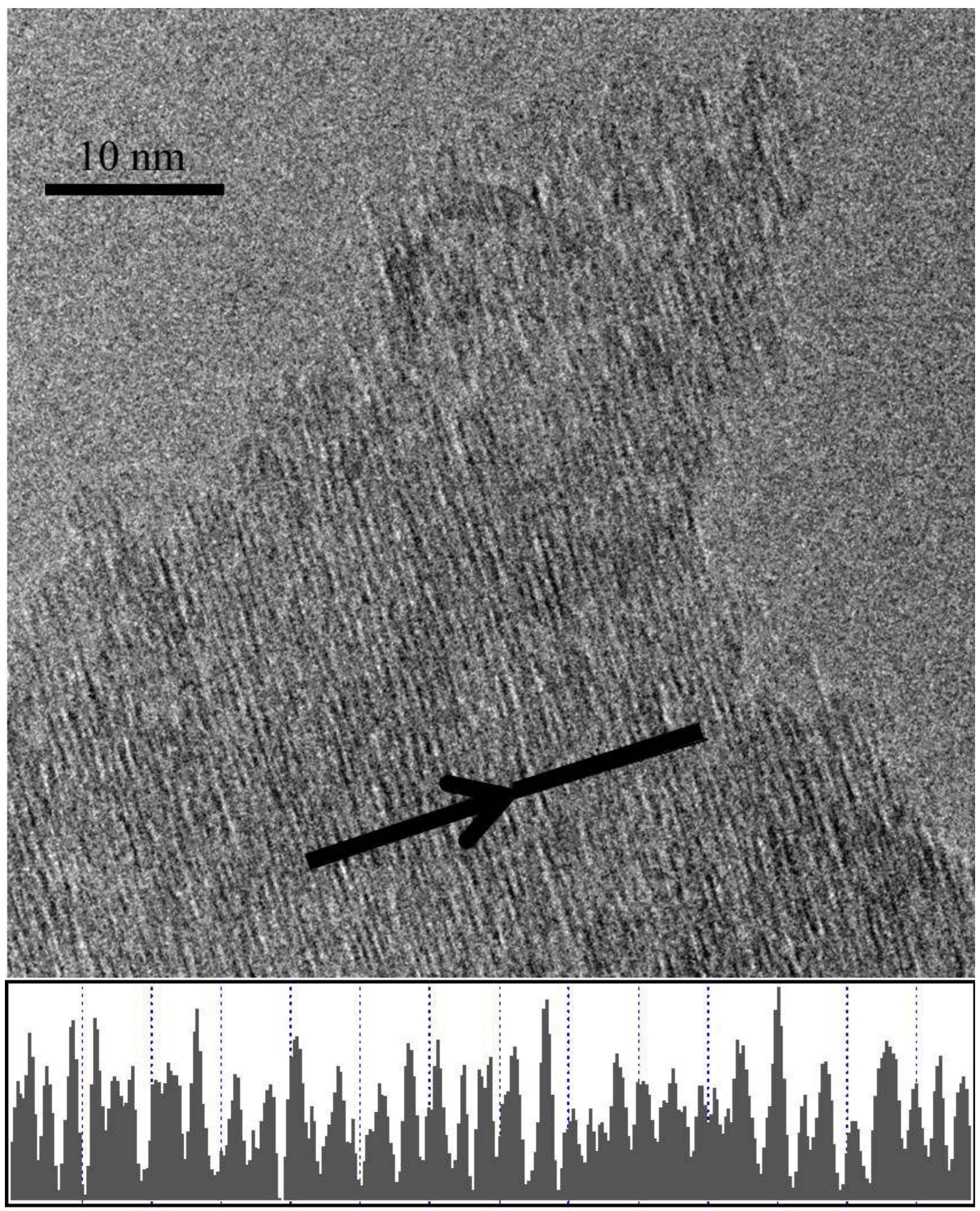


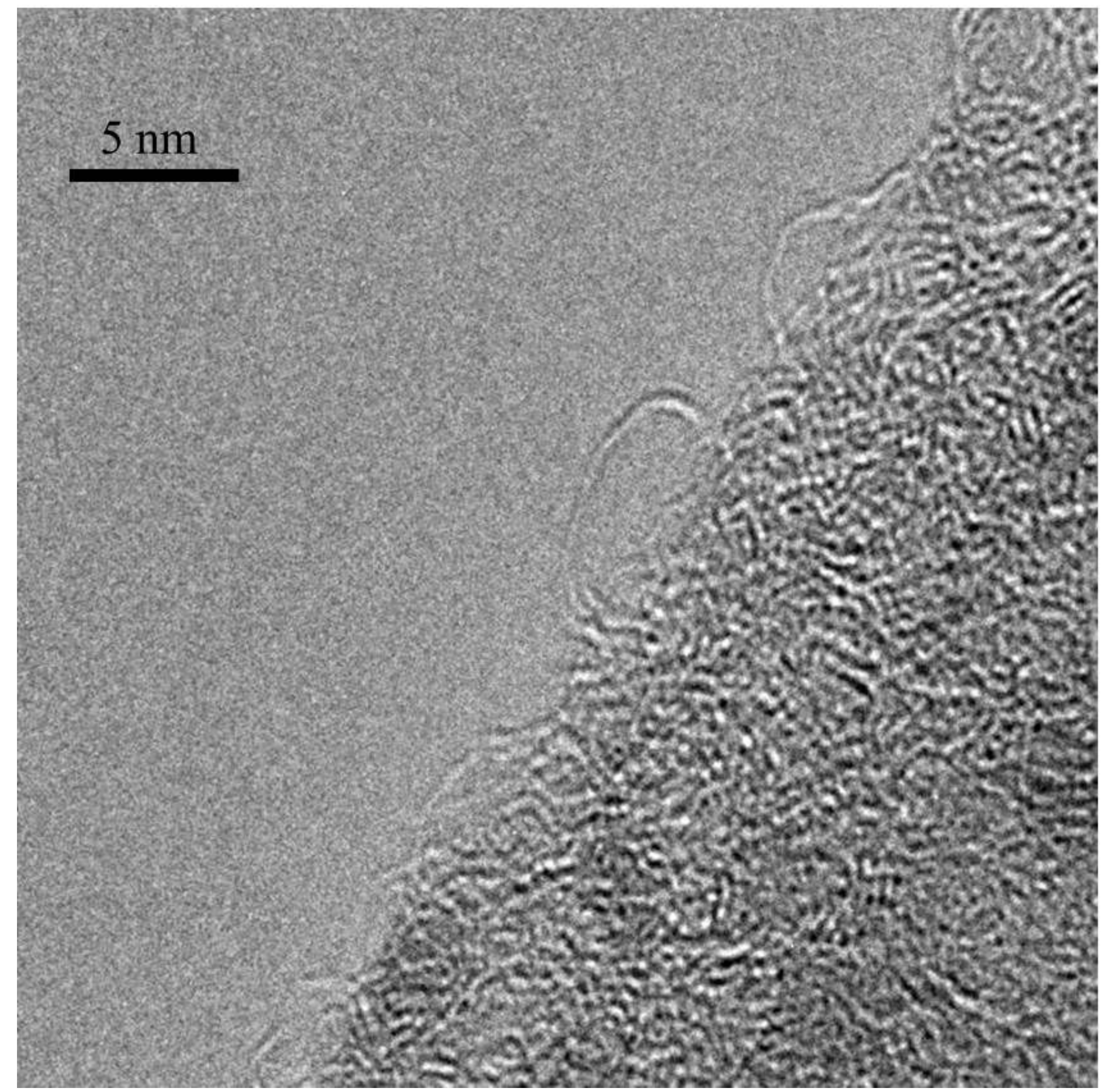
FIG. 2. The relaxed structure of the $(3,0)$ tube, both a doubled unit cell and a space-filling model of the tubular structure.

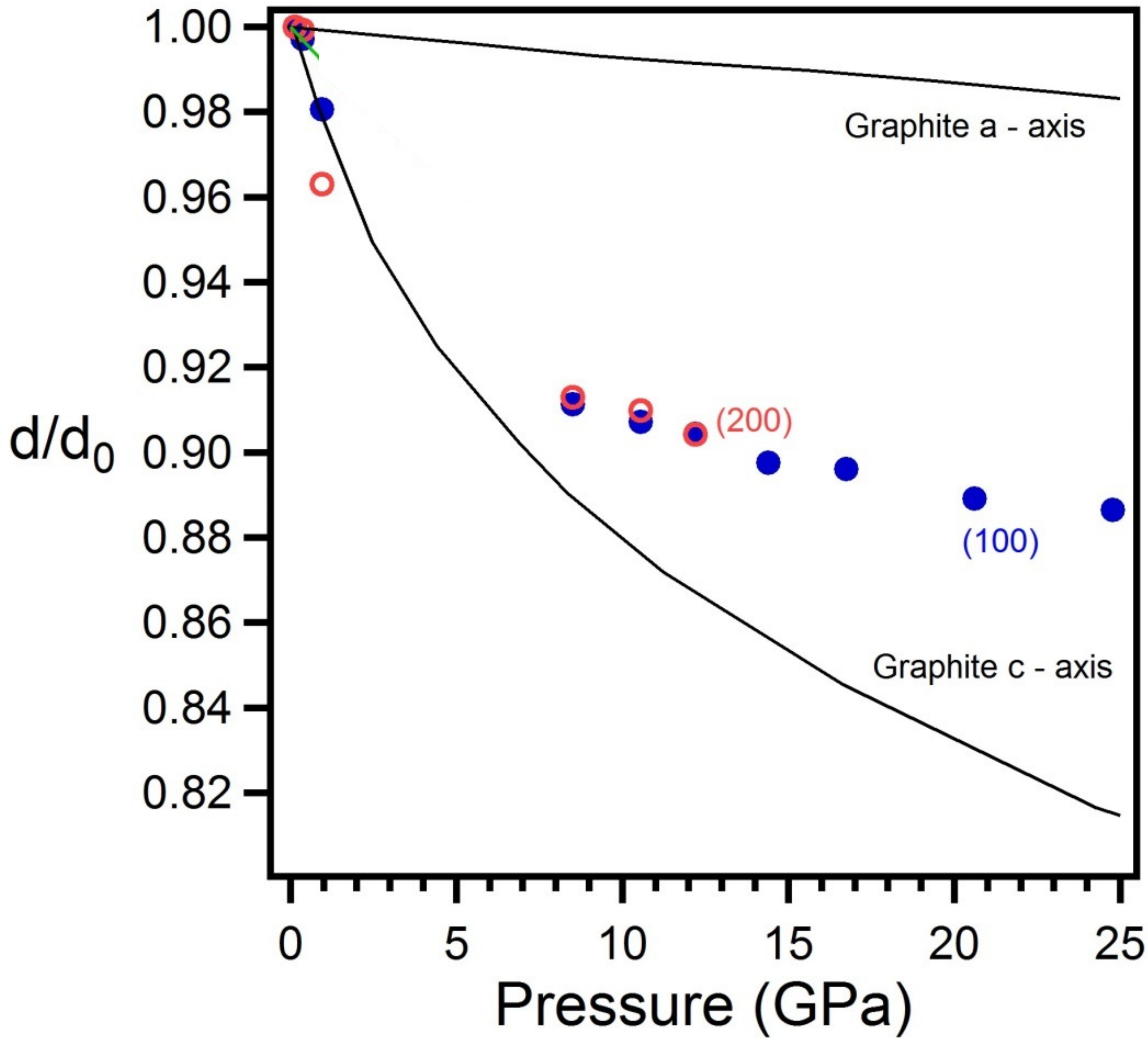
Transmission electron microscopy

as-prepared



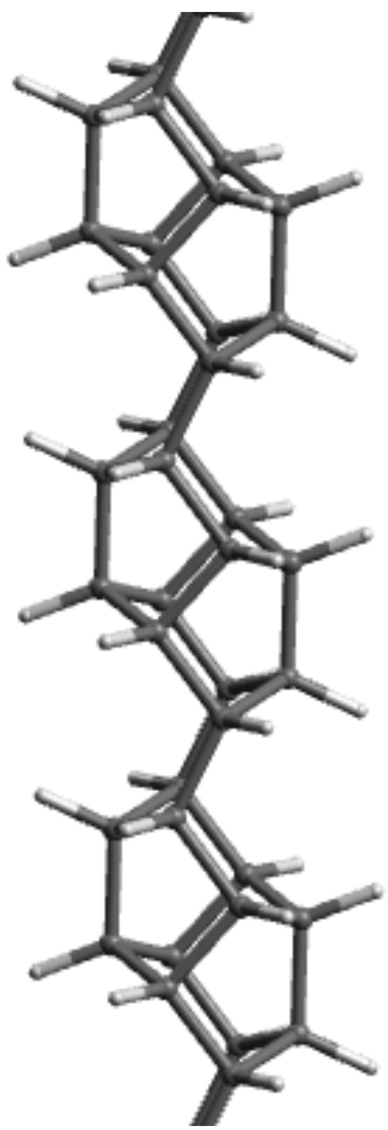
after sonication



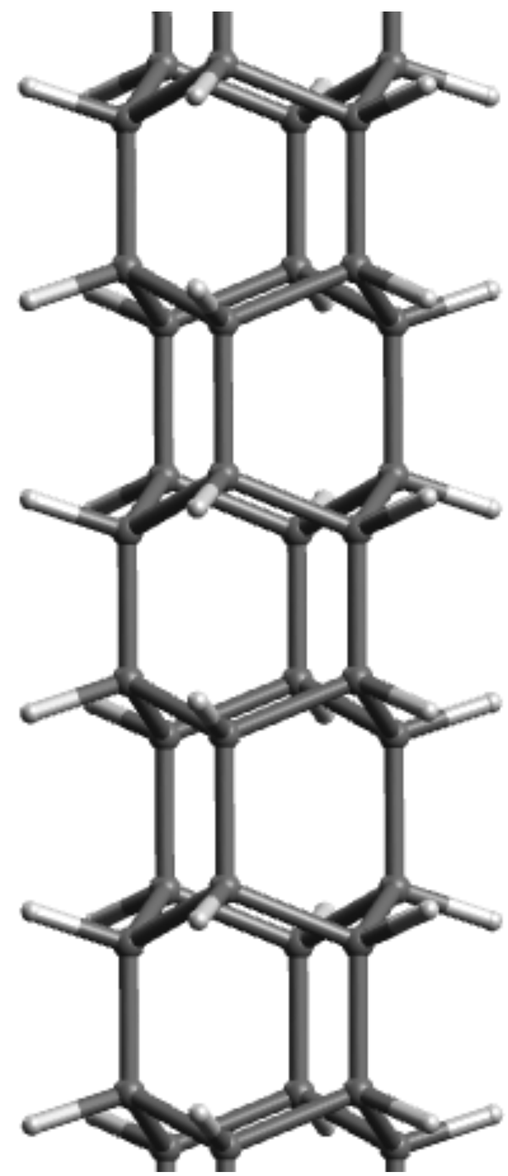


1.00
0.98
0.96
0.94
0.92
0.90
0.88
0.86
0.84
0.82
d/d0
Graphite a - axis
(200)
(100)
Graphite c - axis
0
5
10
15
20
25
Pressure (GPa)

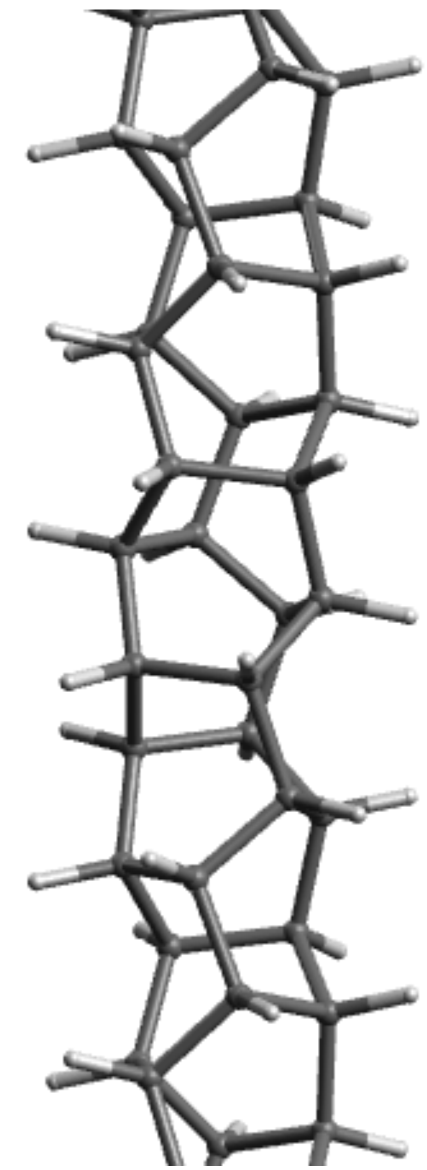
how many ways to make a nanothread?



Polymer I

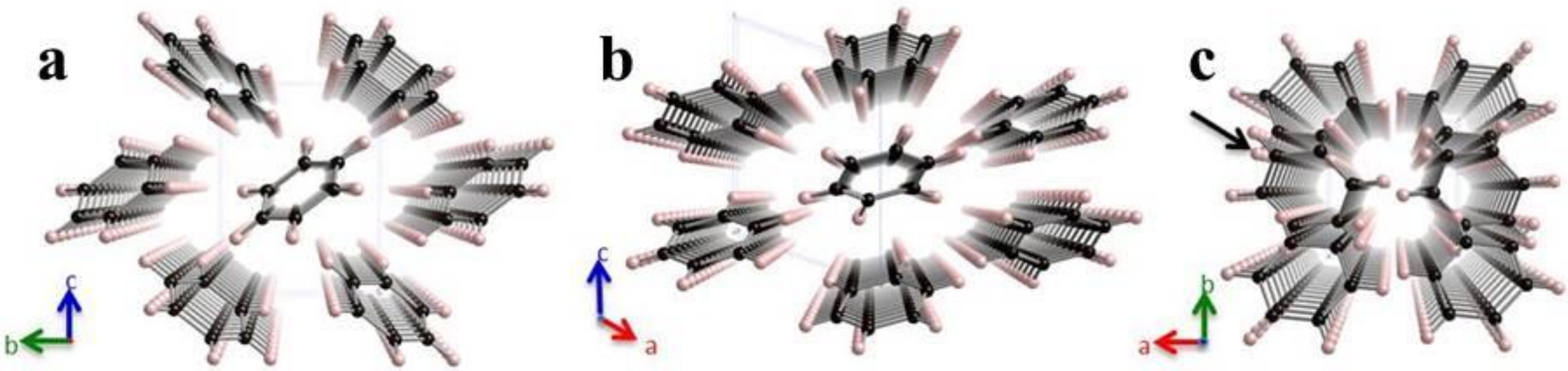


sp^3 tube (3,0)

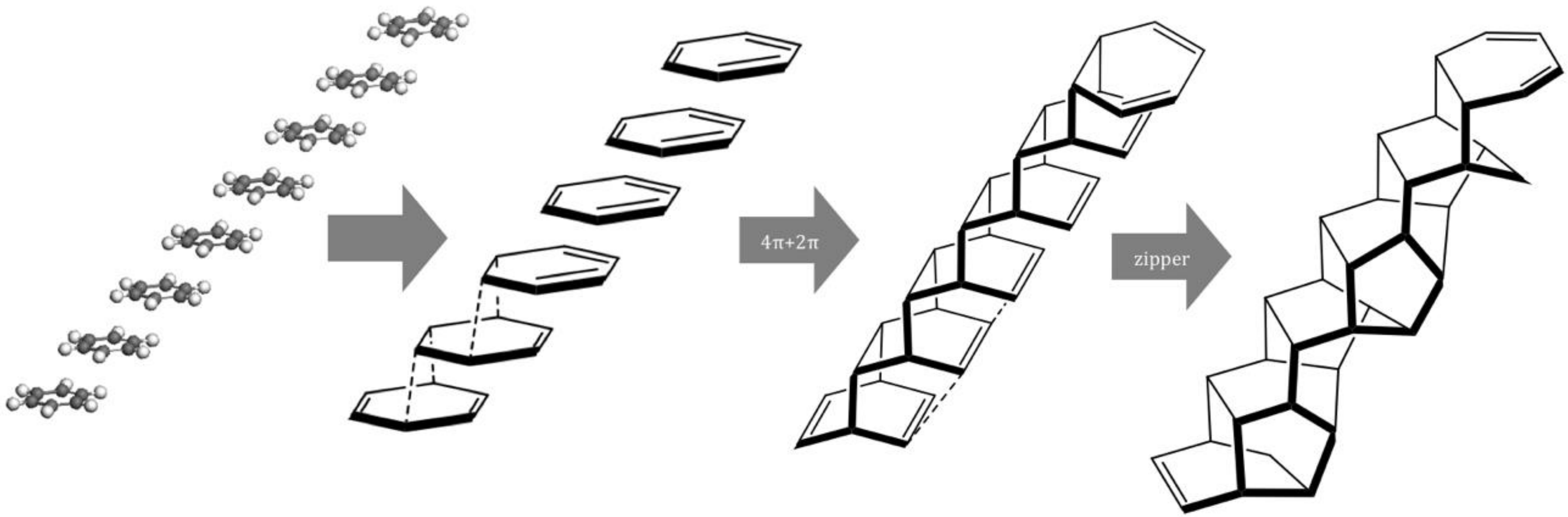


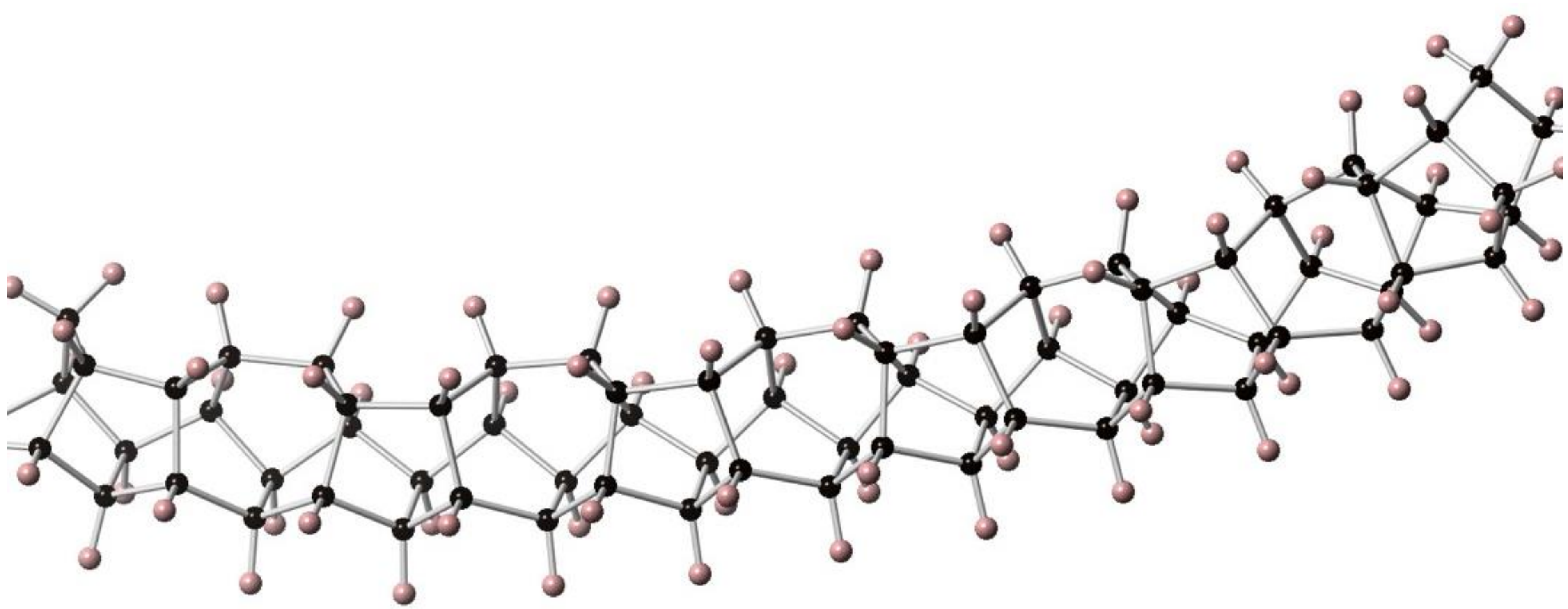
Polytwistane

Columns of stacked benzenes

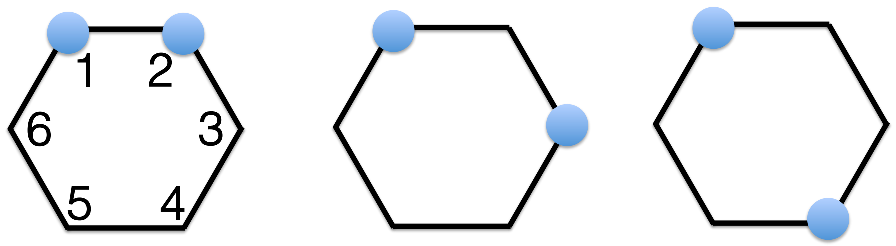


many possible reaction pathways…



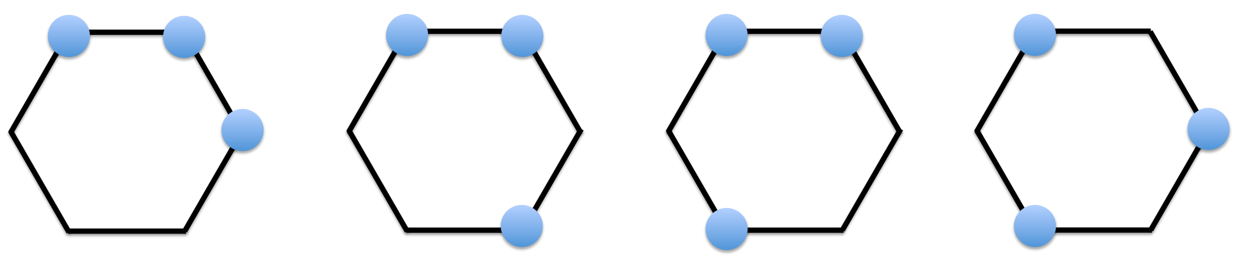


Enumerate



(1, 2) (1, 3) (1, 4)

class II



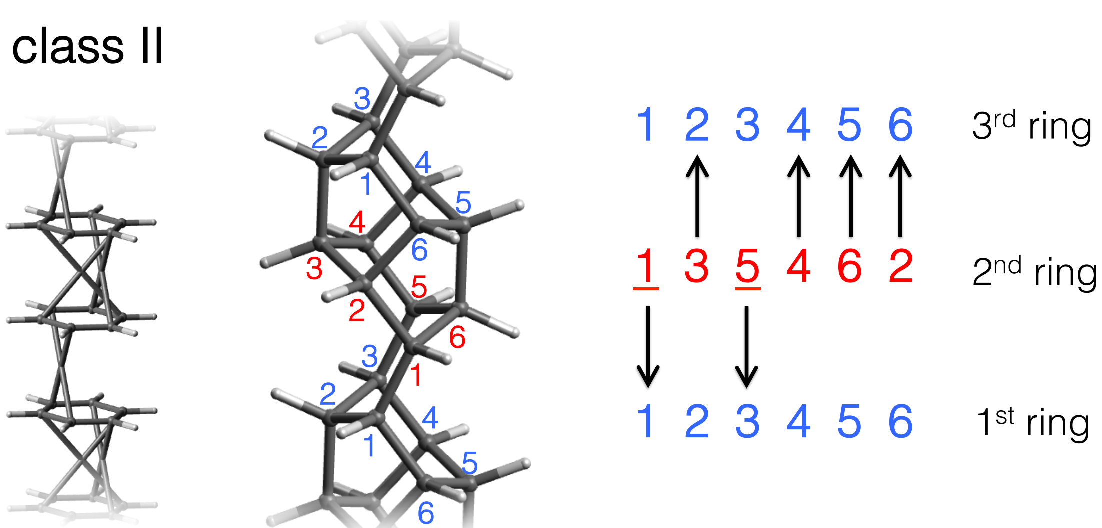
(1, 2, 3) (1, 2, 4) (1, 2, 5) (1, 3, 5)

class III

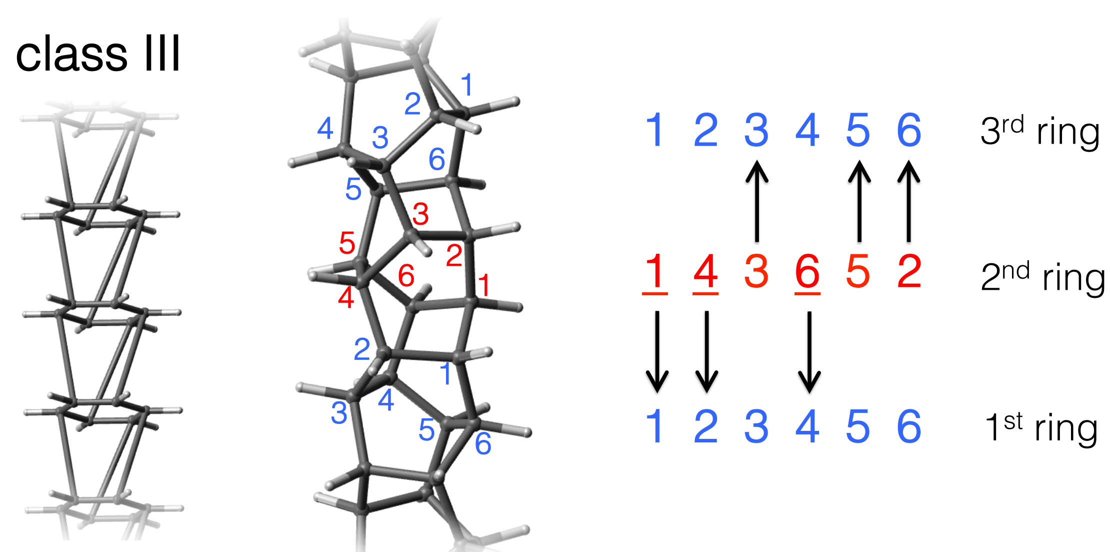
Which atoms bond up?

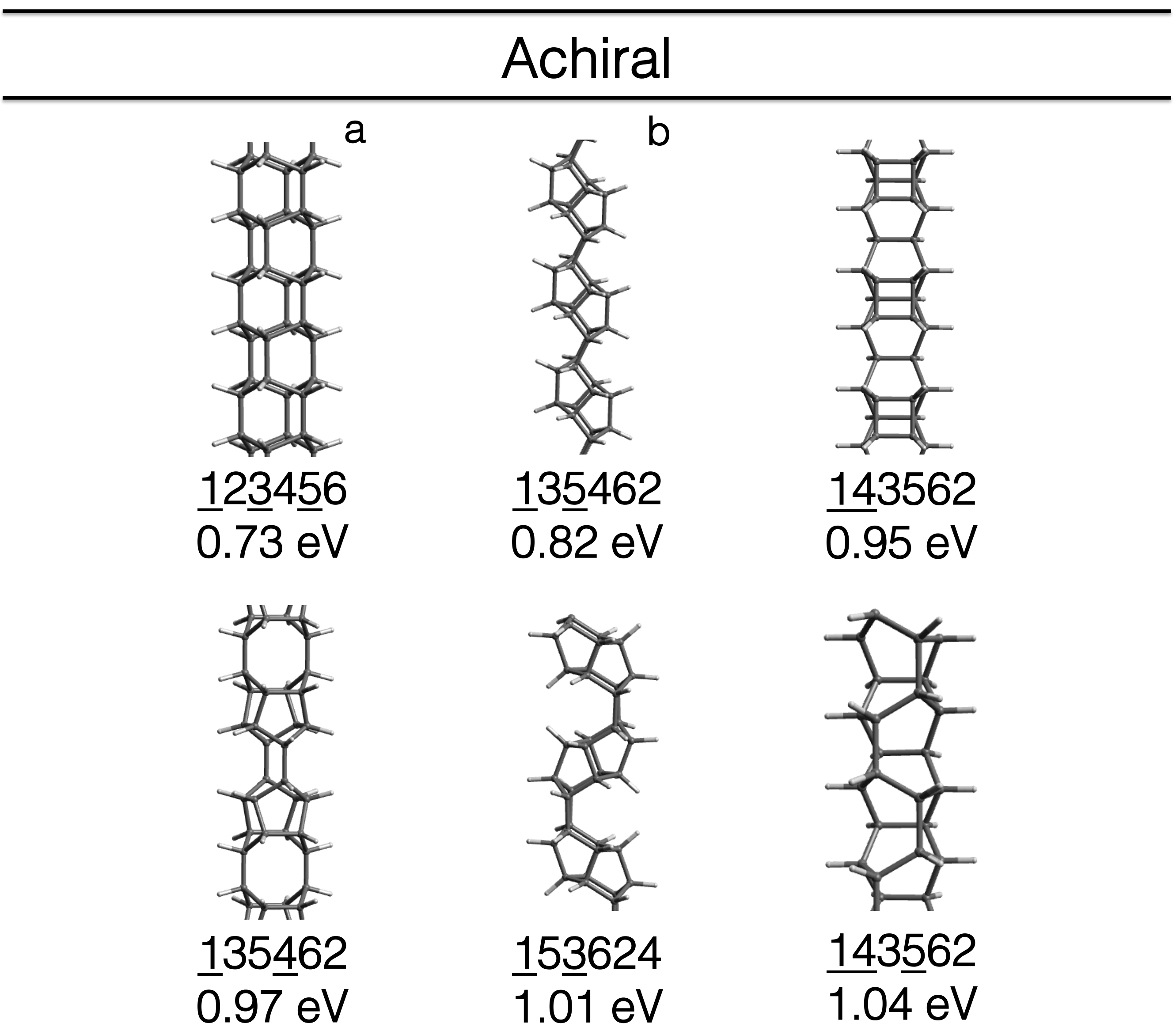
To which atoms in the next ring?

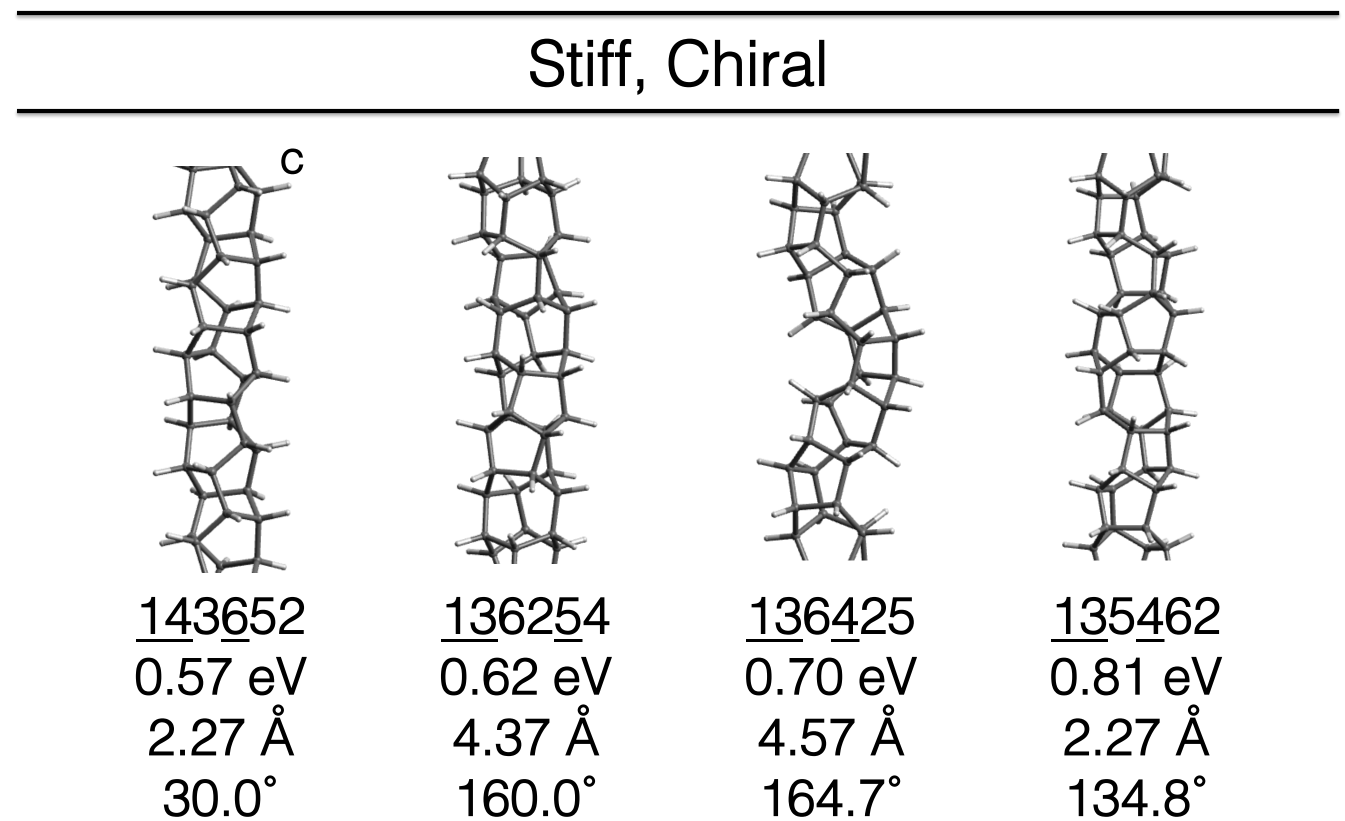
class II

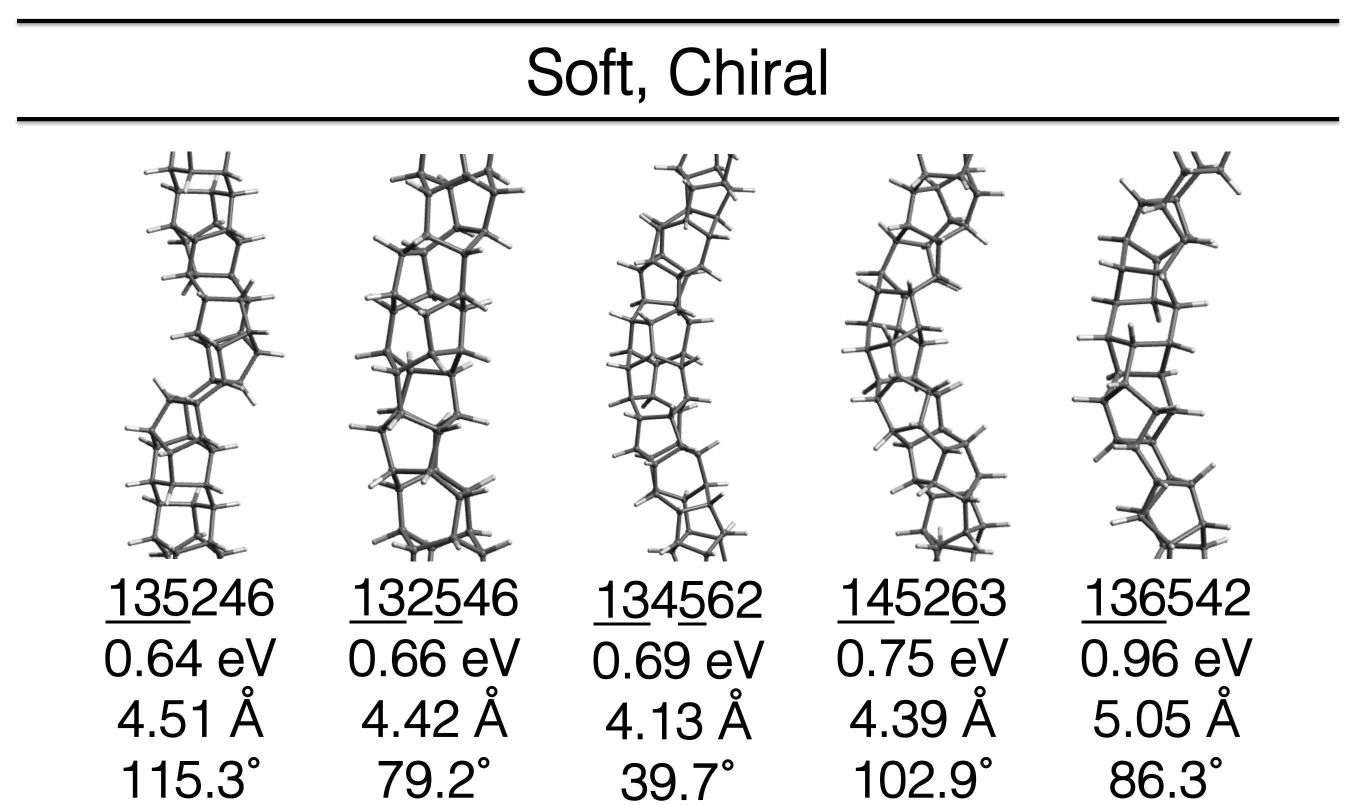


class III



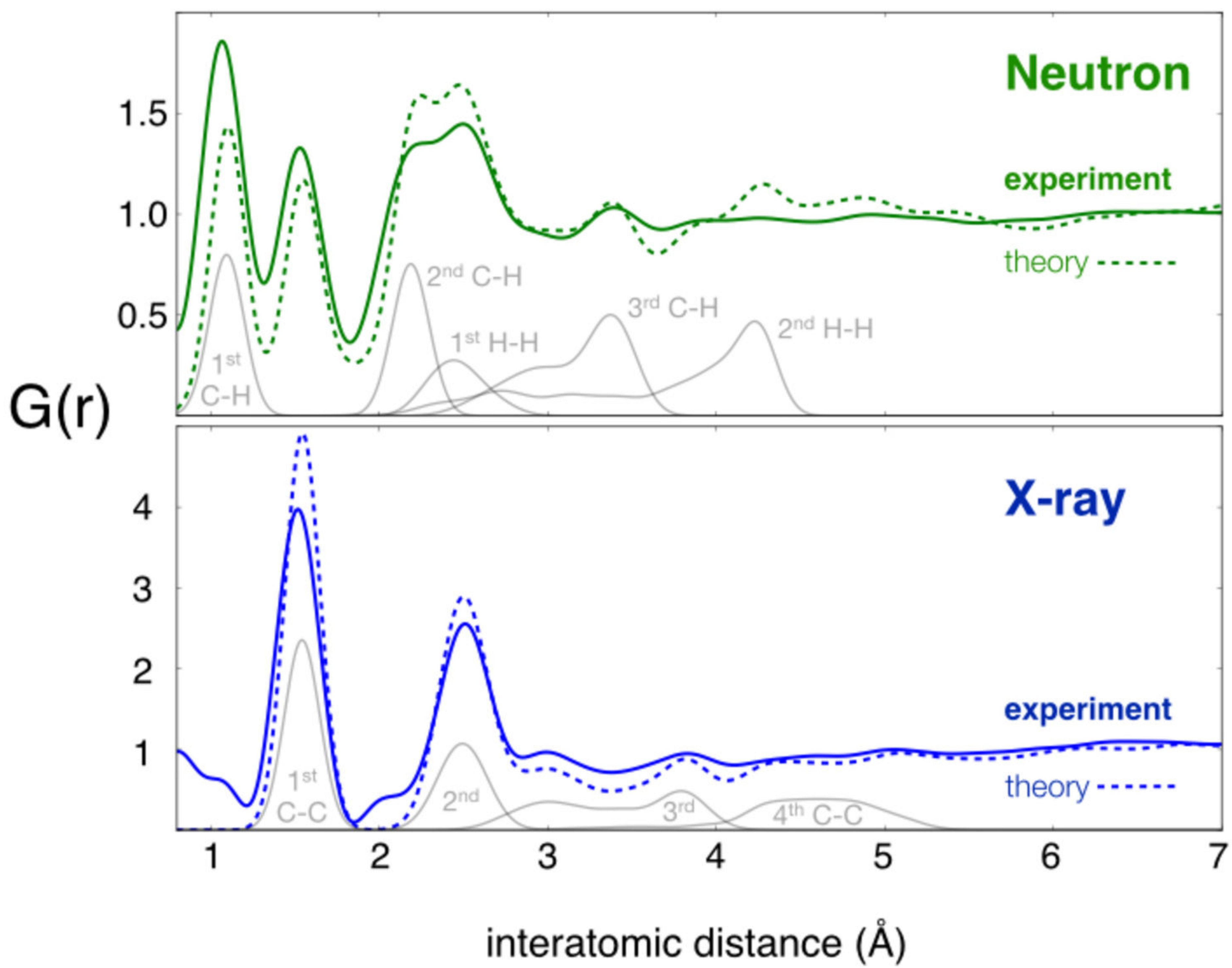


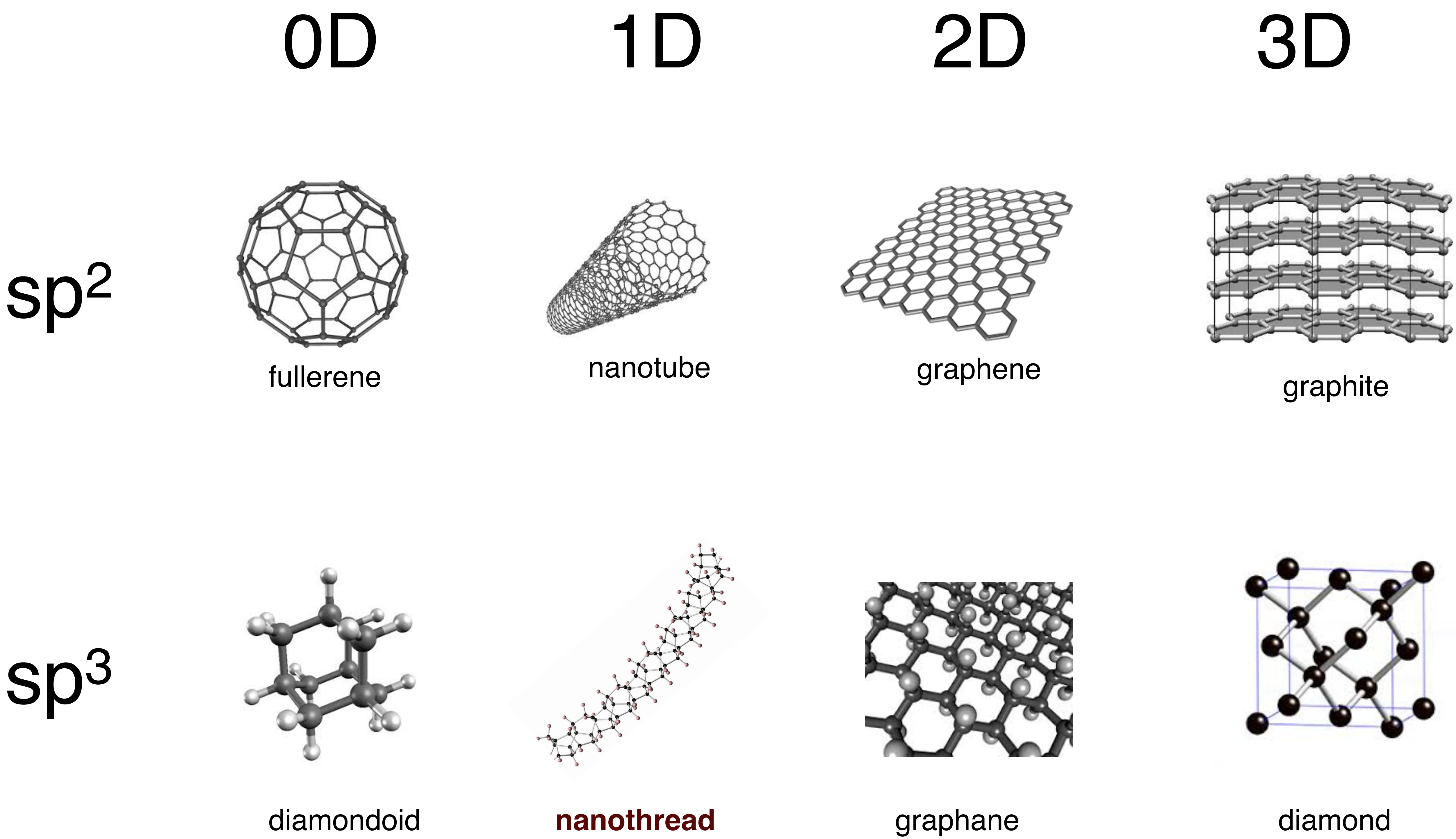




The fifteen lowest-energy nanothreads formed from 1 or 2 rings per topological repeat.

Pair distribution function peaks at sp³ neighbor distances




0D
1D
2D
3D
sp^2
fullerene
nanotube
graphene
graphite
sp^3
diamondoid
nanothread
graphane
diamond

What can we do with them?

Topology		Helical Interpolation				Periodic approximate			
Identifier	Ring Count (n_4, n_5, n_6, n_7, n_8, n_{10})	Energy per $(CH)_6$ eV	Young's Modulus (free, pinned) TPa	λ atoms/Å	Screw (trans., rot.) (Å, °)	R_{eff} Å	E_{gap} eV	n_{C}	$l_{\text{C-C}}$ Å
			Achiral						
$\underline{1}2\underline{3}4\underline{5}6^a$	(0, 0, 6, 0, 0, 0)*	0.73	1.16	2.79	4.30	1.43	3.89	1	$1.54 \cdots 1.57$
$\underline{1}3\underline{5}462^b$	(0, 4, 0, 0, 2, 0)*	0.82	0.98	2.41	4.98	1.40	4.79	4	$1.53 \cdots 1.60$
$\underline{14}3562$	(1, 2, 2, 0, 0, 1)*	0.95	0.93	2.38	5.04	1.40	4.51	4	$1.53 \cdots 1.59$
$\underline{1}35\underline{4}62$	(0, 4, 0, 0, 2, 0)*	0.97	0.90	2.60	9.23	1.41	4.55	3	$1.54 \cdots 1.58$
$\underline{1}5\underline{3}624$	(0, 4, 1, 0, 0, 1)	1.01	0.59	2.60	9.22	1.69	4.48	4	$1.53 \cdots 1.59$
$\underline{14}3\underline{5}62$	(0, 2, 2, 2, 0, 0)*	1.04	1.08	2.44	4.91	1.35	4.11	4	$1.51 \cdots 1.67$
			Stiff, chiral						
$\underline{14}3\underline{6}52^c$	(0, 0, 6, 0, 0, 0)*	0.57	(1.11, 1.14)	2.45	(0.82, 130.0)	1.29	3.52	2	$1.54 \cdots 1.57$
$\underline{13}62\underline{5}4$	(0, 2, 2, 2, 0, 0)*	0.62	(0.73, 0.74)	2.75	(4.37, 160.0)	1.97	4.27	12	$1.53 \cdots 1.58$
$\underline{13}6\underline{4}25$	(0, 2, 3, 0, 1, 0)	0.70	(0.64, 0.64)	2.63	(4.57, 164.7)	1.88	4.28	12	$1.53 \cdots 1.57$
$\underline{13}5\underline{4}62$	(0, 4, 0, 0, 2, 0)	0.81	(0.63, 0.76)	2.64	(2.27, 134.8)	1.58	4.55	6	$1.54 \cdots 1.57$
			Soft, chiral						
$\underline{135}246$	(0, 4, 0, 0, 2, 0)*	0.64	(0.31, 0.37)	2.66	(4.51, 115.3)	2.31	4.23	12	$1.53 \cdots 1.58$
$\underline{13}2\underline{5}46$	(0, 2, 2, 2, 0, 0)*	0.66	(0.35, 0.37)	2.72	(4.42, 79.2)	2.10	4.16	12	$1.53 \cdots 1.58$
$\underline{13}4\underline{5}62$	(0, 2, 2, 2, 0, 0)*	0.69	(0.08, 0.10)	2.91	(4.13, 39.7)	4.09	4.53	12	$1.53 \cdots 1.58$
$\underline{14}52\underline{6}3$	(0, 2, 2, 2, 0, 0)*	0.75	(0.19, 0.26)	2.74	(4.39, 102.9)	2.44	4.19	12	$1.53 \cdots 1.58$
$\underline{136}524$	(0, 2, 2, 2, 0, 0)	0.96	(0.41, 0.45)	2.38	(5.05, 86.3)	2.26	4.24	12	$1.54 \cdots 1.59$

(some slides omitted for confidentiality)

Nanothreads

- intermediate between polymer & nanowire
- all-surface sp^3
- does it work with multi-ring aromatics?
- how far can we lower the synthesis pressure?