

به نام خدا



مرکز دانلود رایگان
مهندسی متالورژی و مواد

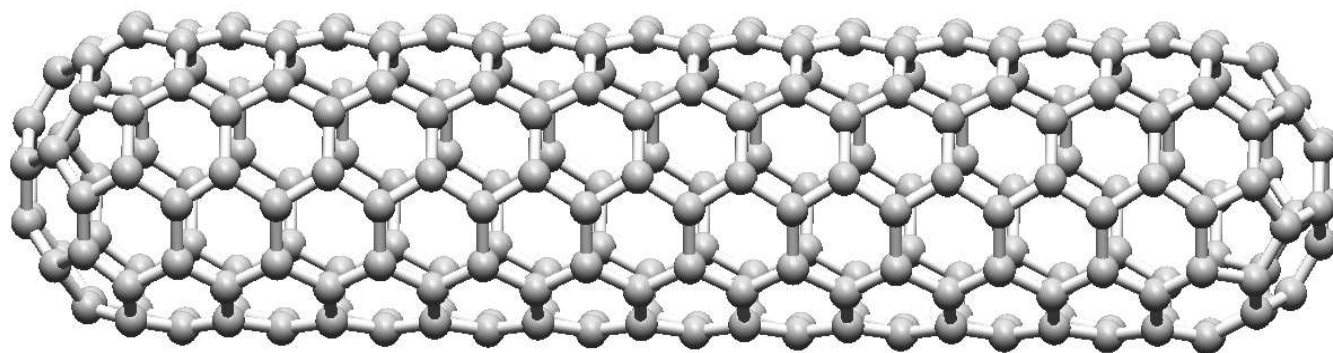
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Steffen Weber's

Crystallography Picture Book

Nanotubes & Nanocones

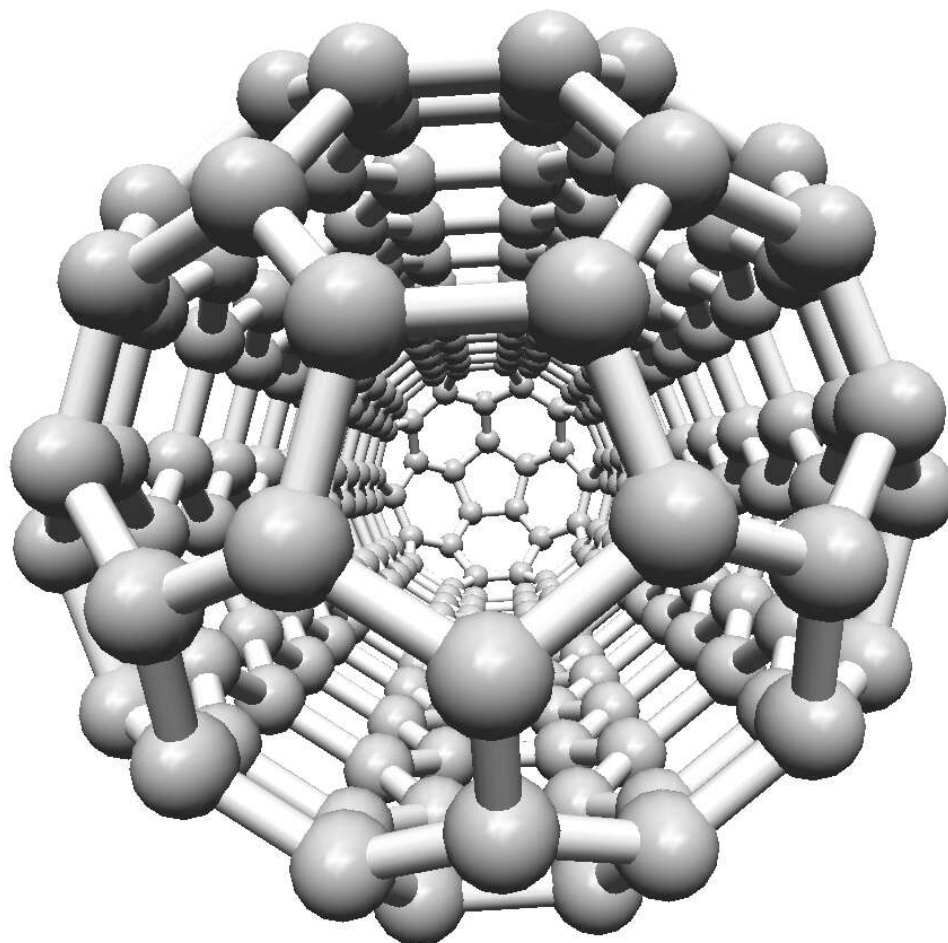


Preface

This is the first in a series of picture books that I plan to create for educational purposes. All images in this volume were created using the program *NanotubeModeler* from JCrystalSoft. A free version of this program can be downloaded at www.jcrystal.com. My earliest implementation of routines for the creation and visualization of nanotubes and nanocones was realized in JSV (Java Structure Viewer), a program which I wrote while working at NIRIM in Japan. Later I wrote a Java Applet version on the request of Dr. Jeremy Sloan. This year I finally wrote *NanotubeModeler* as a stand-alone Windows application on the request of my former colleague Dr. Paul Dennig who is now working for Ahwahnee Technology. The nano-geometries are created by first generating a flat graphene sheet and then rolling it into a tube or a cone. Two types of nanotubes can be capped with parts of the well-known Buckyball (C_{60}). These are the $\{5,5\}$ and the $\{9,0\}$ tubes, which have a suitable diameter of about 6.9 Å. Nanotubes are identified by their chiral indices $\{m,n\}$. One distinguishes between armchair structures ($n=m$), zig-zag structures ($n=0$) and chiral structures. Nanocones are characterized by the disclination angle, which corresponds to the part that is removed from the flat sheet before rolling it into a cone.

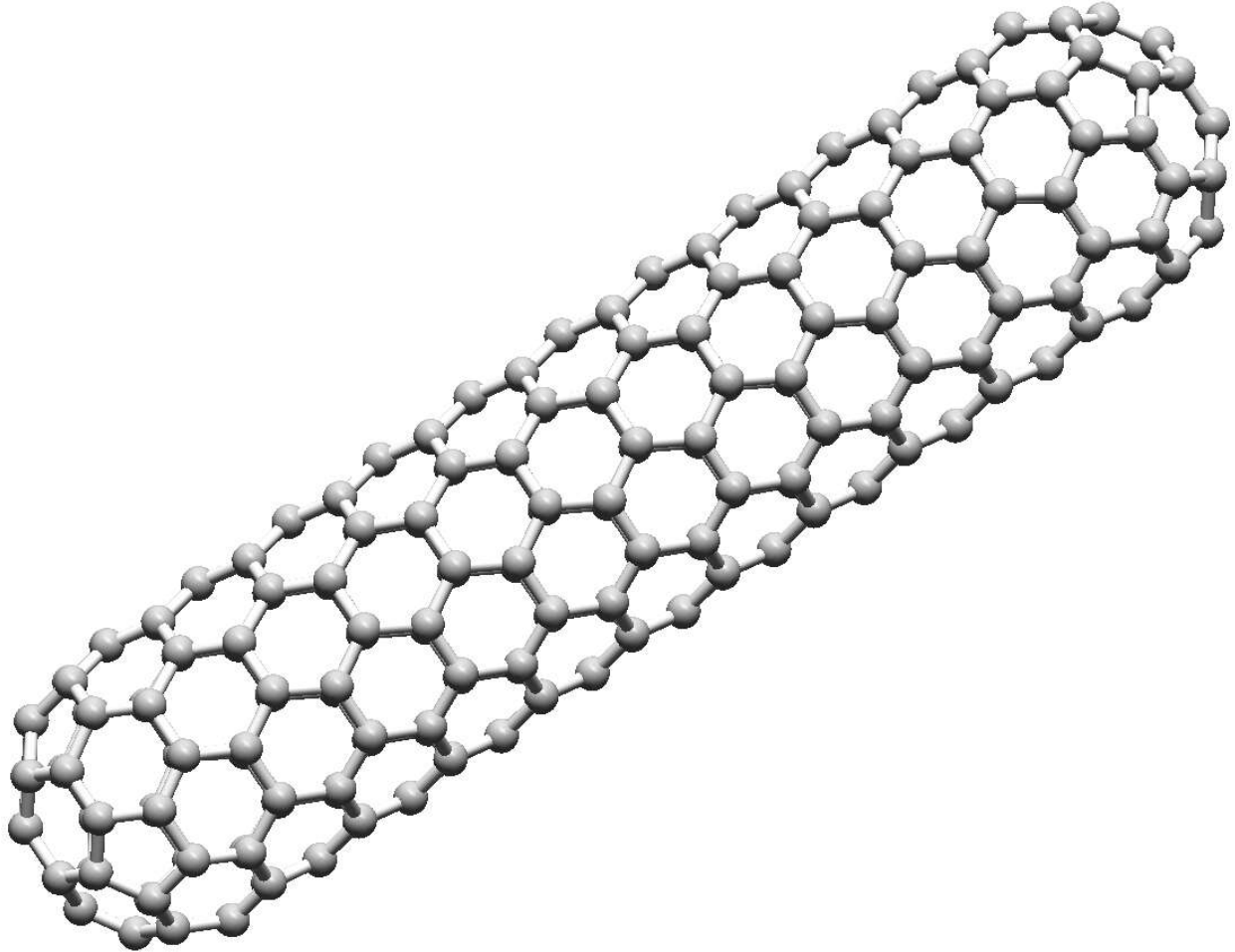
Steffen Weber, Ph.D.
December 10, 2004
Livermore, California
www.jcrystal.com/steffenweber

Capped {5,5} Tube



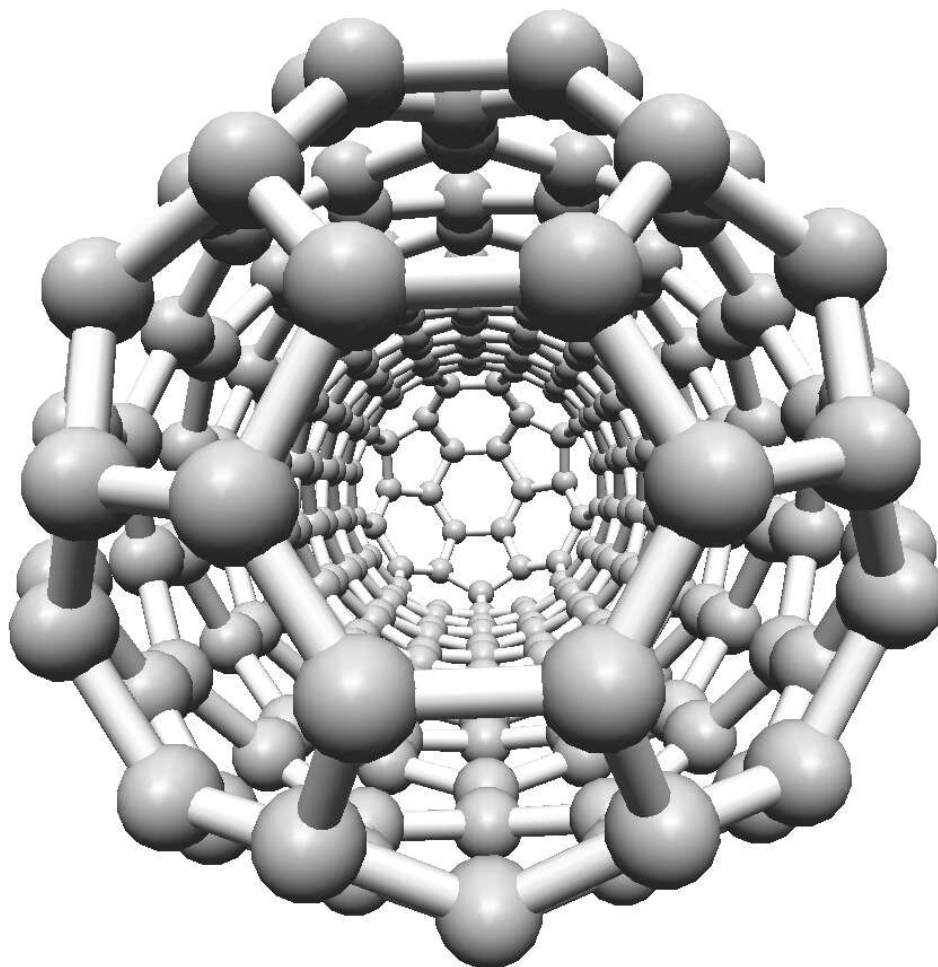
Carbon Nanotube
Armchair structure with Bucky-ball caps

Capped {5,5} Tube



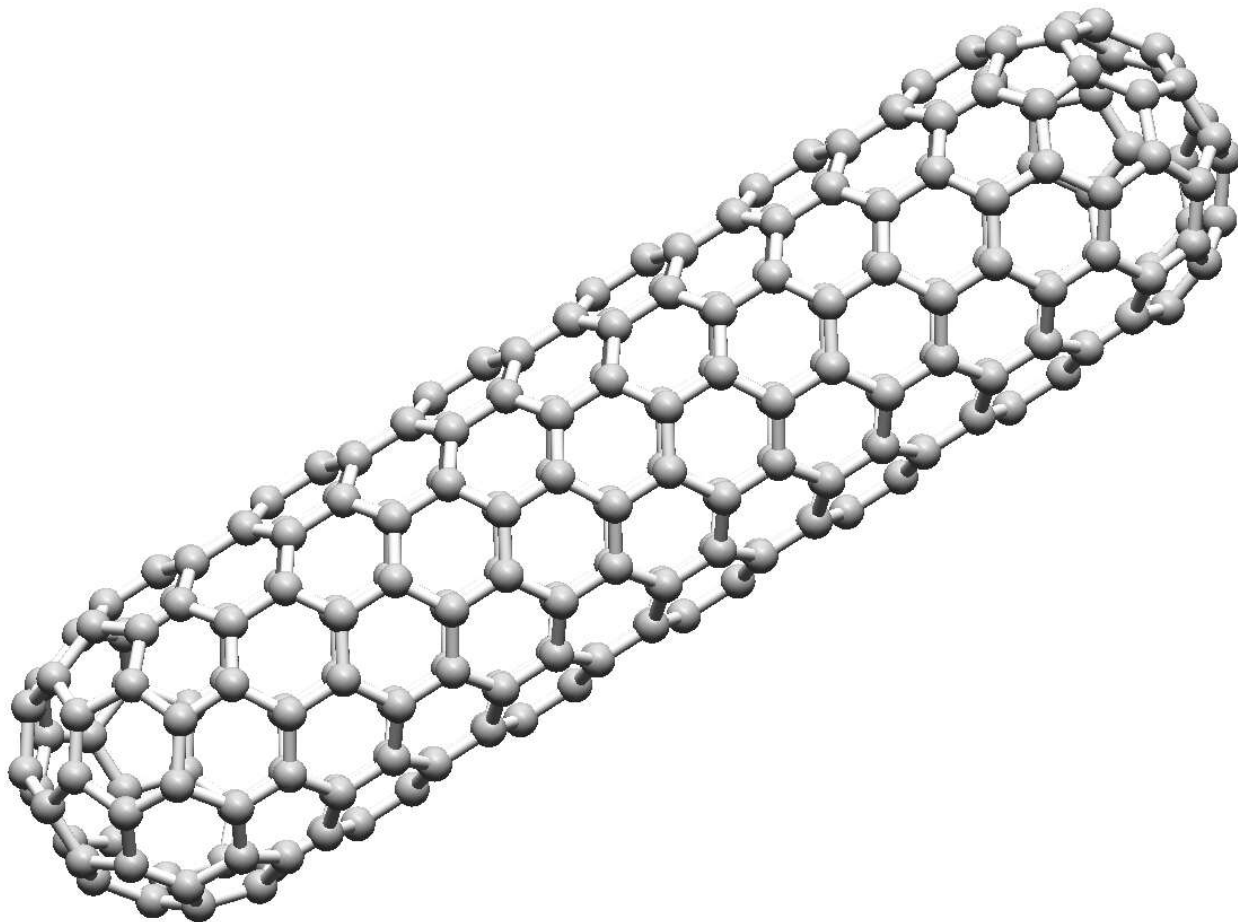
Carbon Nanotube
Armchair structure with Bucky-ball caps
Length ~ 25 Å, Diameter ~ 6.75 Å

Capped {9,0} Tube



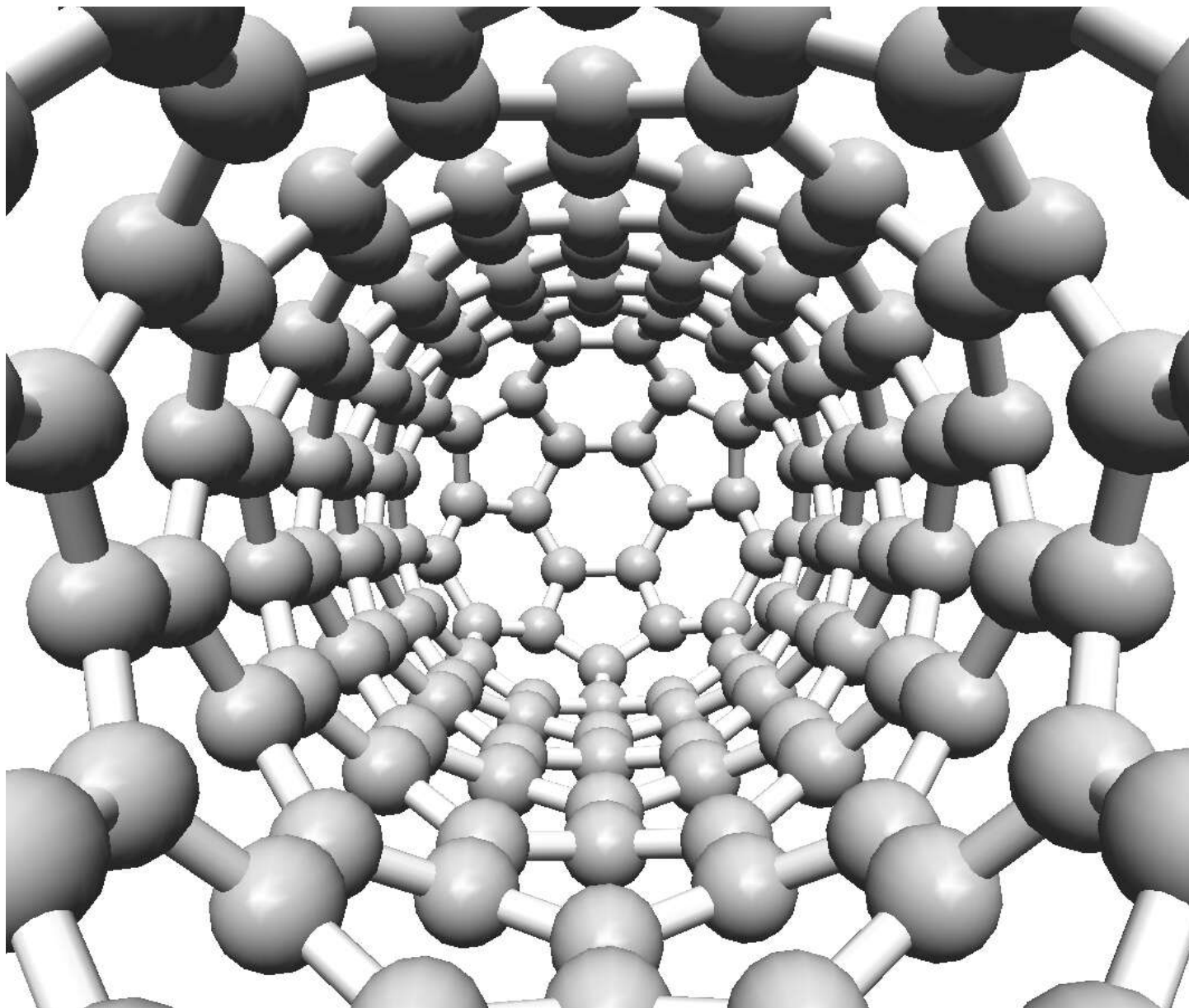
Carbon Nanotube
Zigzag structure with Bucky-ball caps

Capped {9,0} Tube



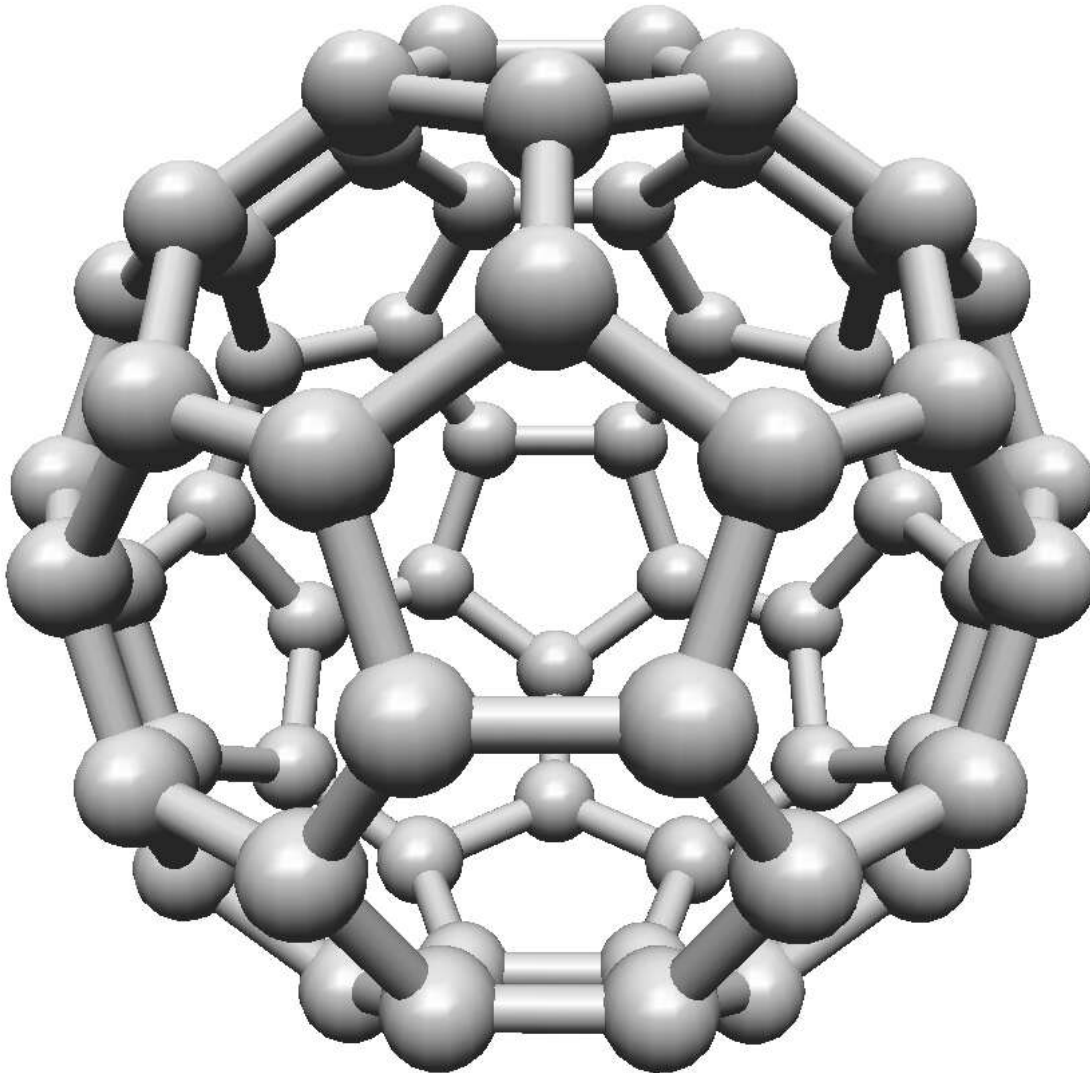
Carbon Nanotube
Armchair structure with Bucky-ball caps
Length $\sim 25 \text{ \AA}$, Diameter $\sim 6.99 \text{ \AA}$

Inside Capped {9,0} Tube



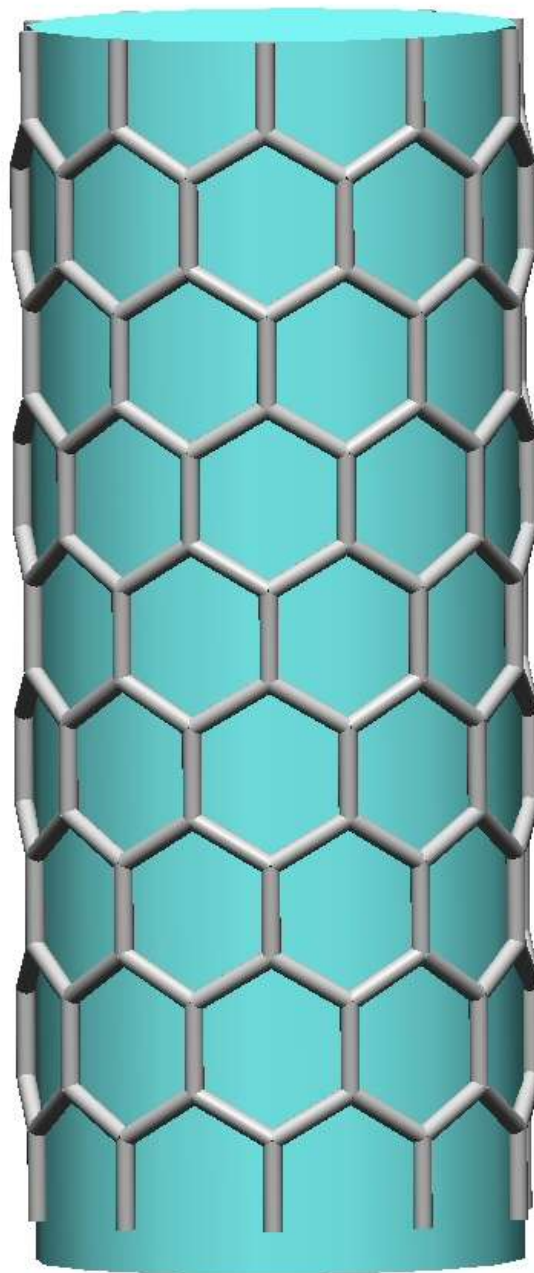
Inside a capped {9,0} nanotube

Bucky-Ball (C₆₀)



A Buckyball, the well-known Fullerene with icosahedral symmetry. Two different sections of the Buckyball can be used to cap the {5,5} and {9,0} nanotubes.

$\{10,0\}$ Nanotube



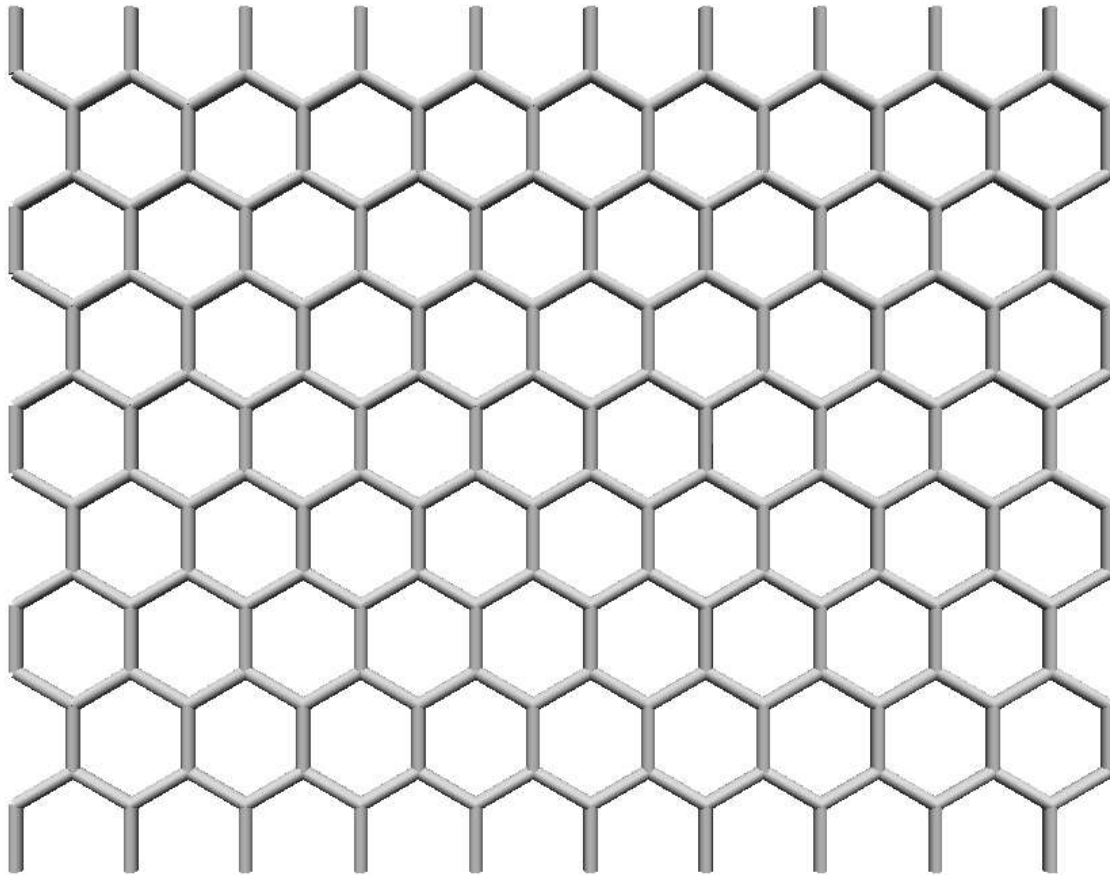
Zig-zag structure
Length $\sim 19 \text{ \AA}$, Diameter $\sim 7.77 \text{ \AA}$

$\{10,10\}$ Nanotube



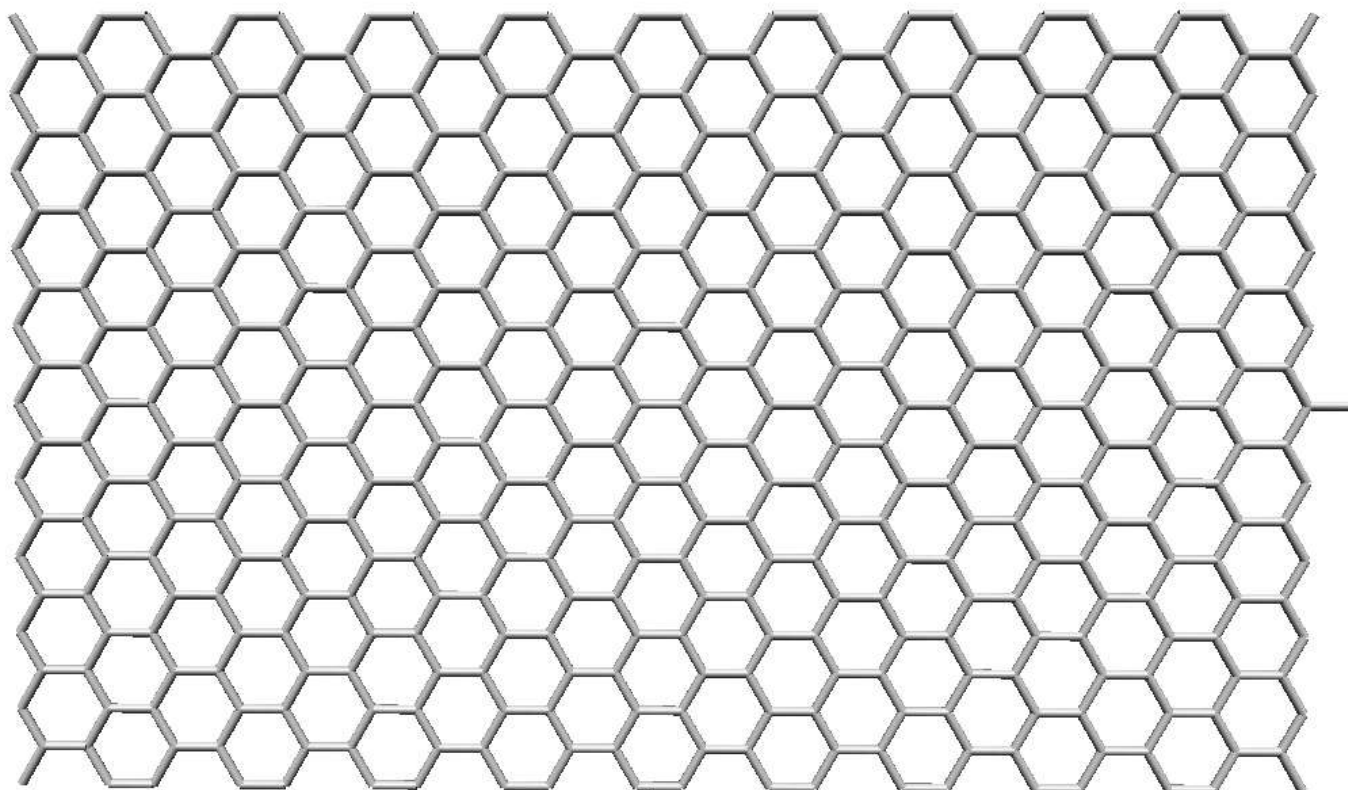
Armchair structure
Length $\sim 25 \text{ \AA}$, Diameter $\sim 13.465 \text{ \AA}$

$\{10,0\}$ Graphene Sheet



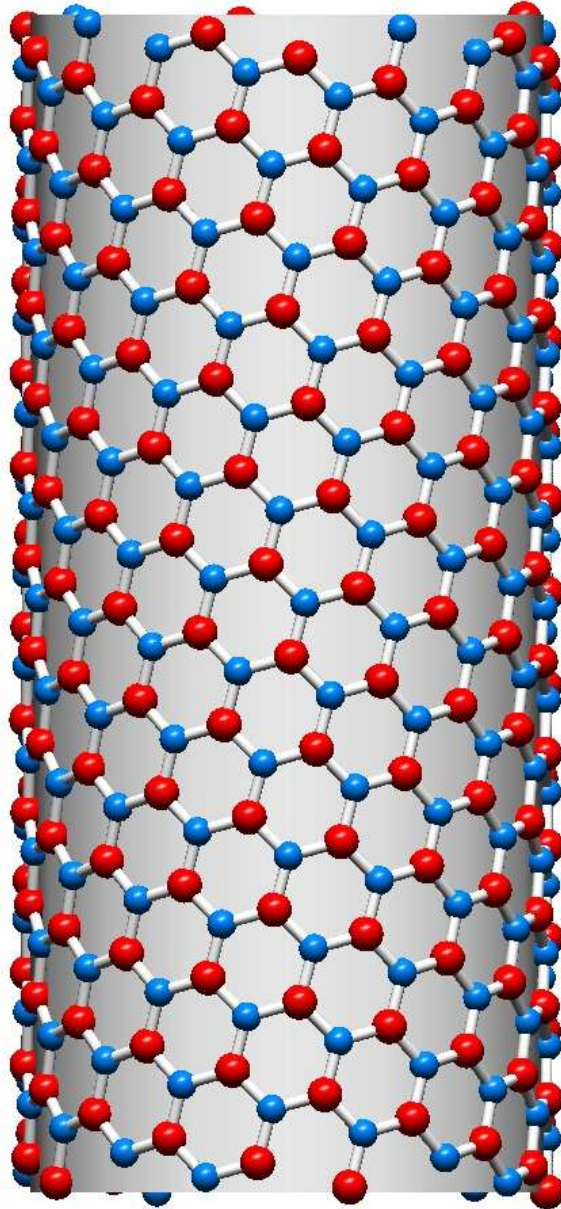
Zig-zag structure
This sheet can be rolled into a $\{10,0\}$ nanotube

$\{10,10\}$ Graphene Sheet



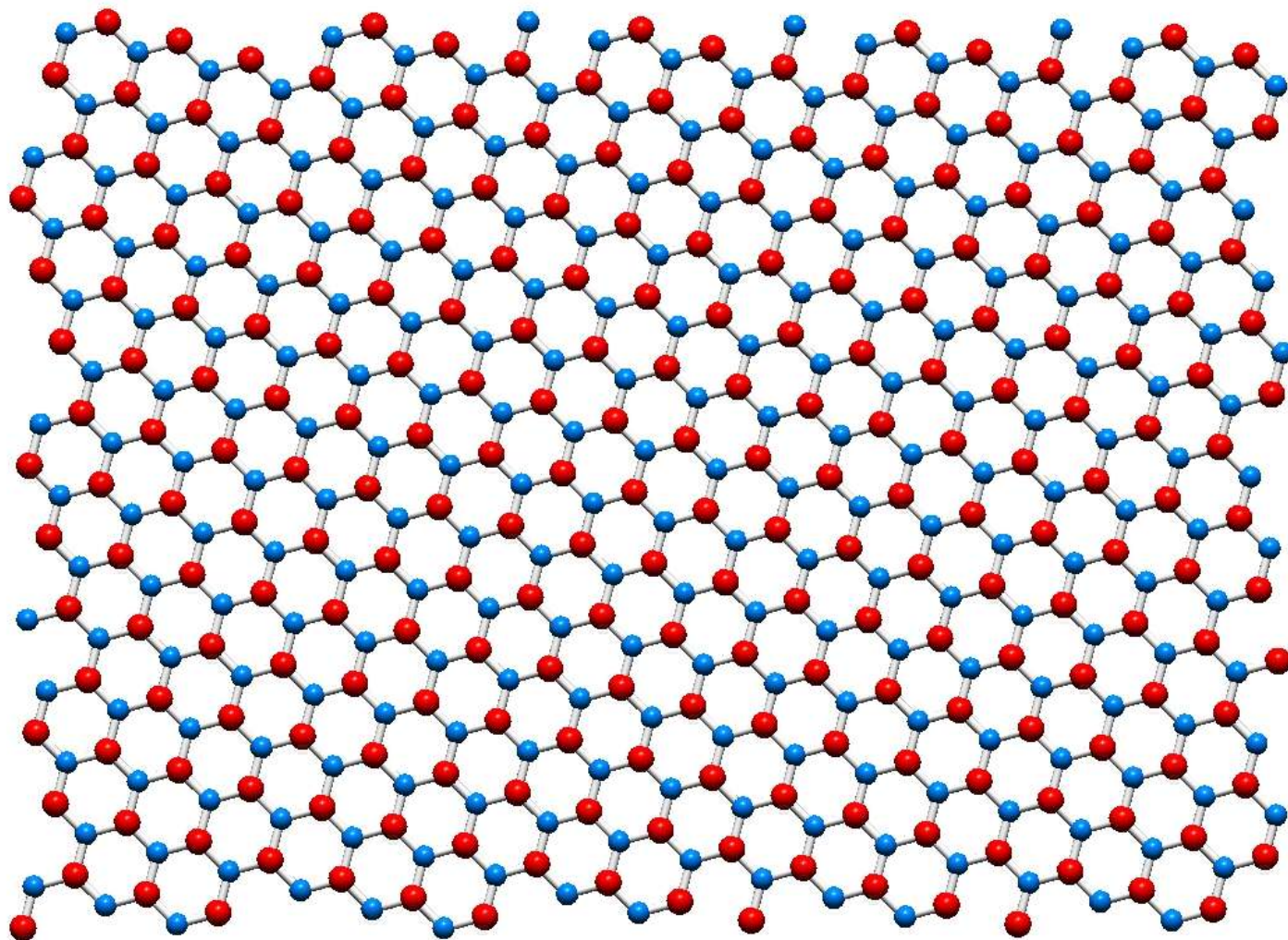
Armchair structure
This sheet can be rolled into a $\{10,10\}$ nanotube

{14,5} BN-Nanotube



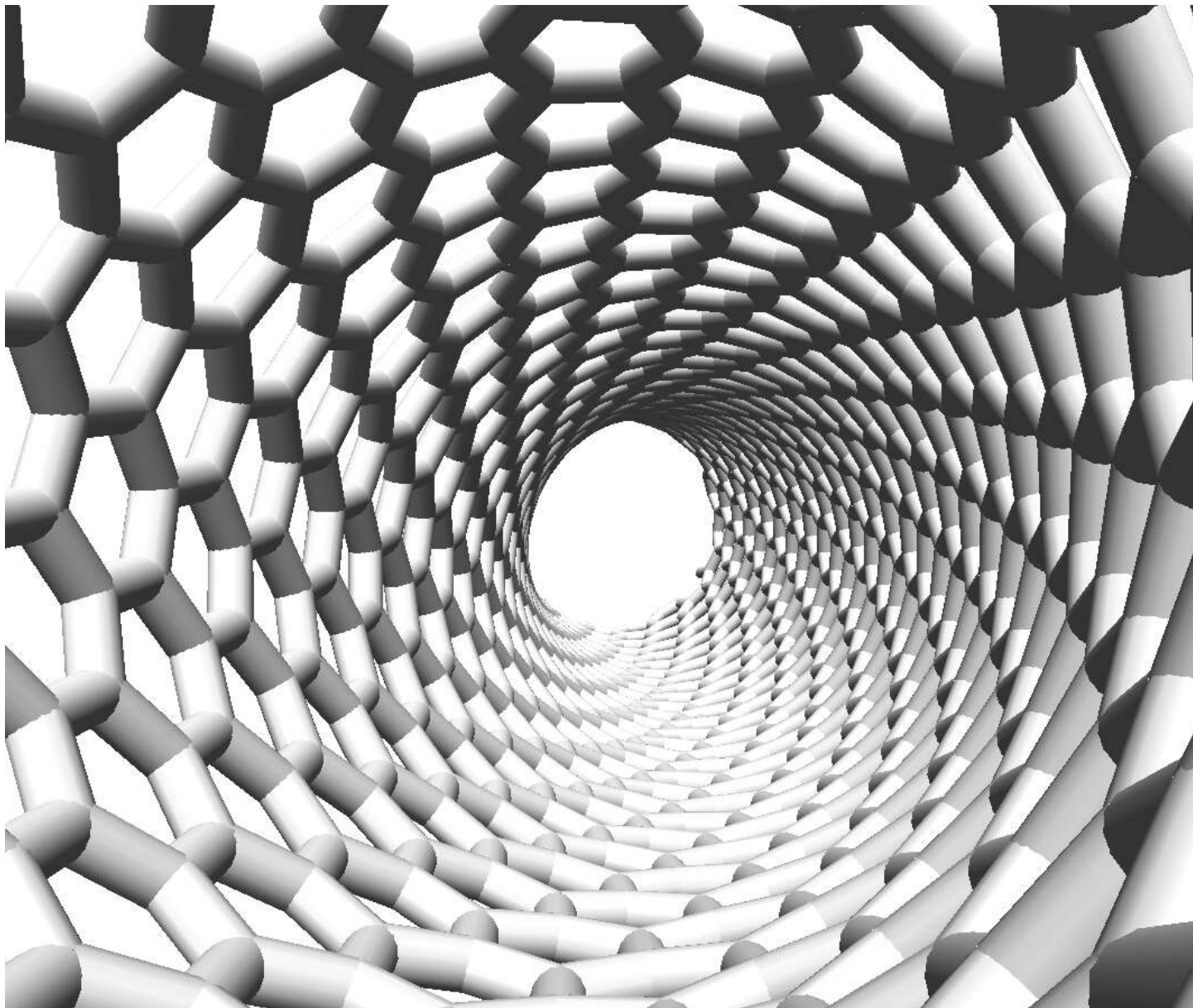
Chiral Boron-Nitride nanotube
Length $\sim 30 \text{ \AA}$, Diameter $\sim 13.26 \text{ \AA}$

{14,5} BN-Sheet



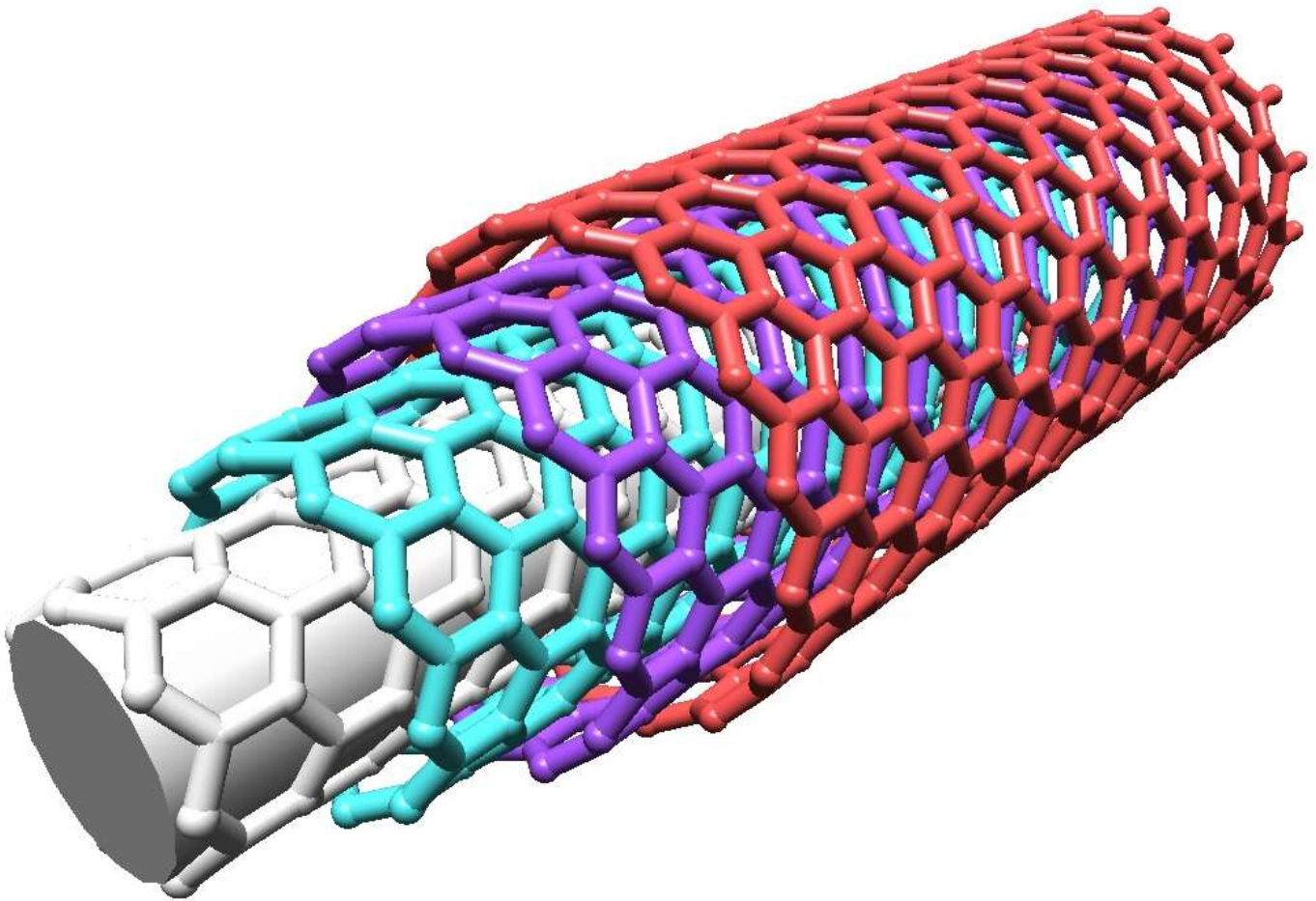
Chiral structure
This sheet can be rolled into a {14,5} nanotube

Inside {14,5} Nanotube



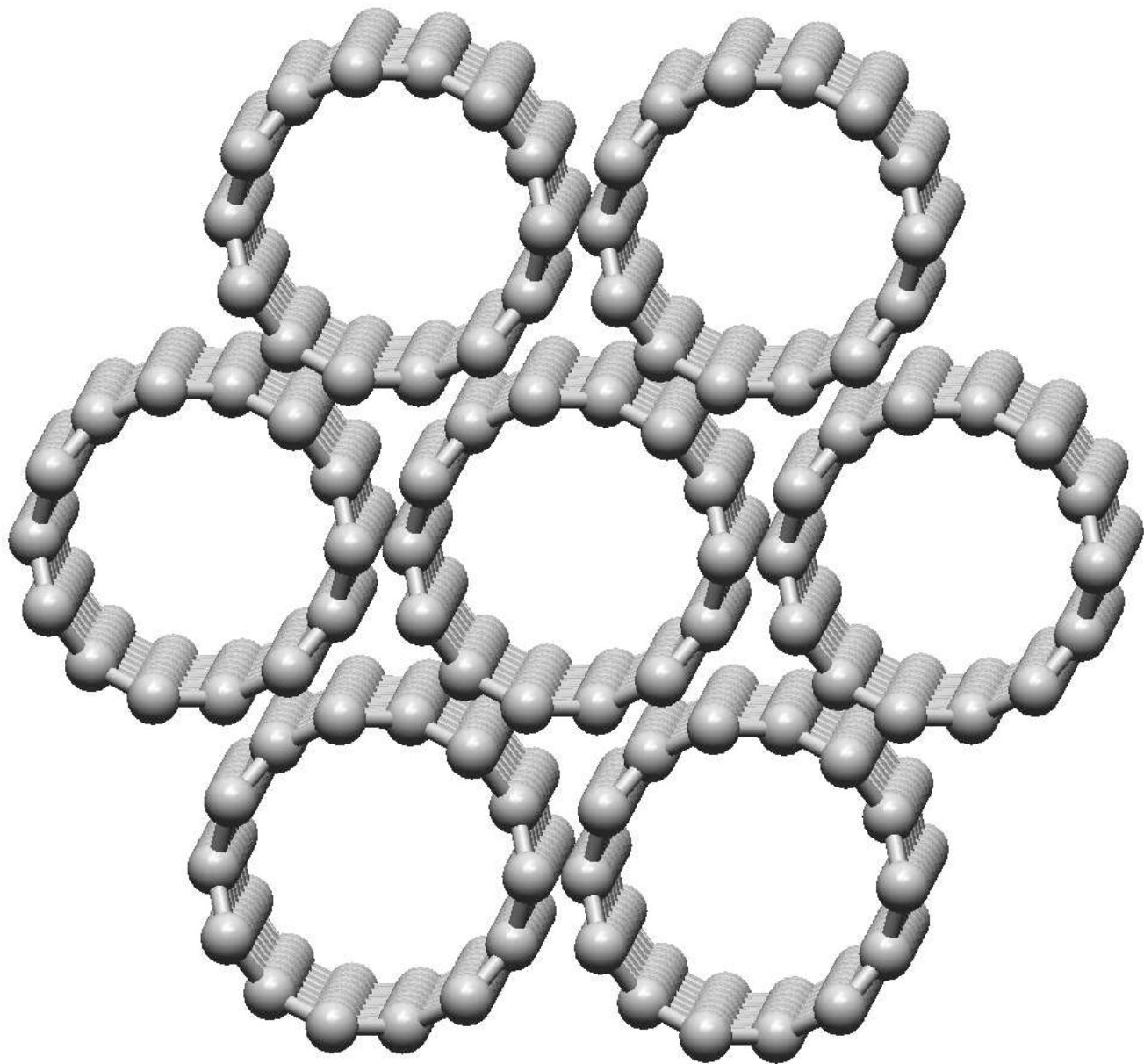
Inside a bent {14,5} nanotube

MWCNT



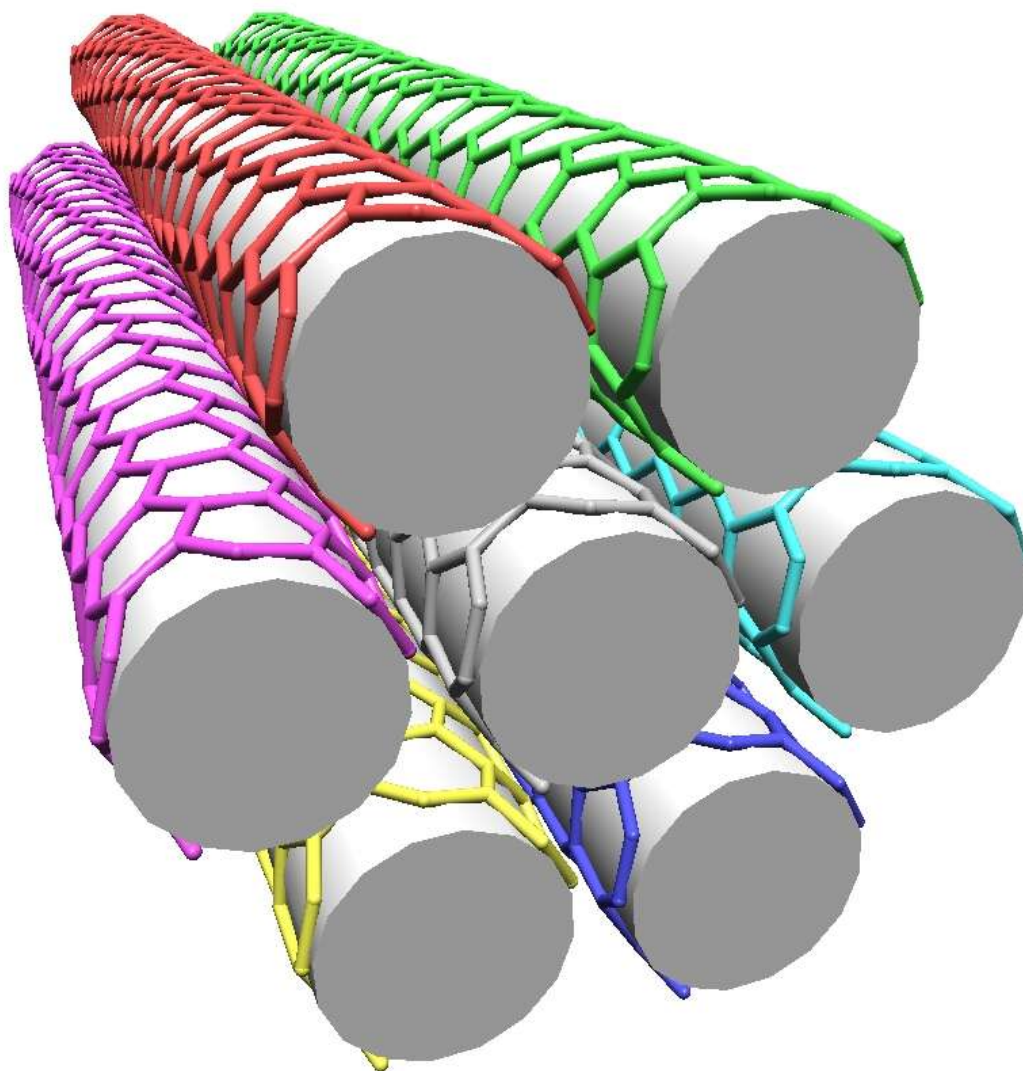
A multi-walled carbon nanotube (MWCNT)
{7,0}, {10,0}, {13,0} and {16,0} tubes

$\{7,0\}$ Nanotube Bundle



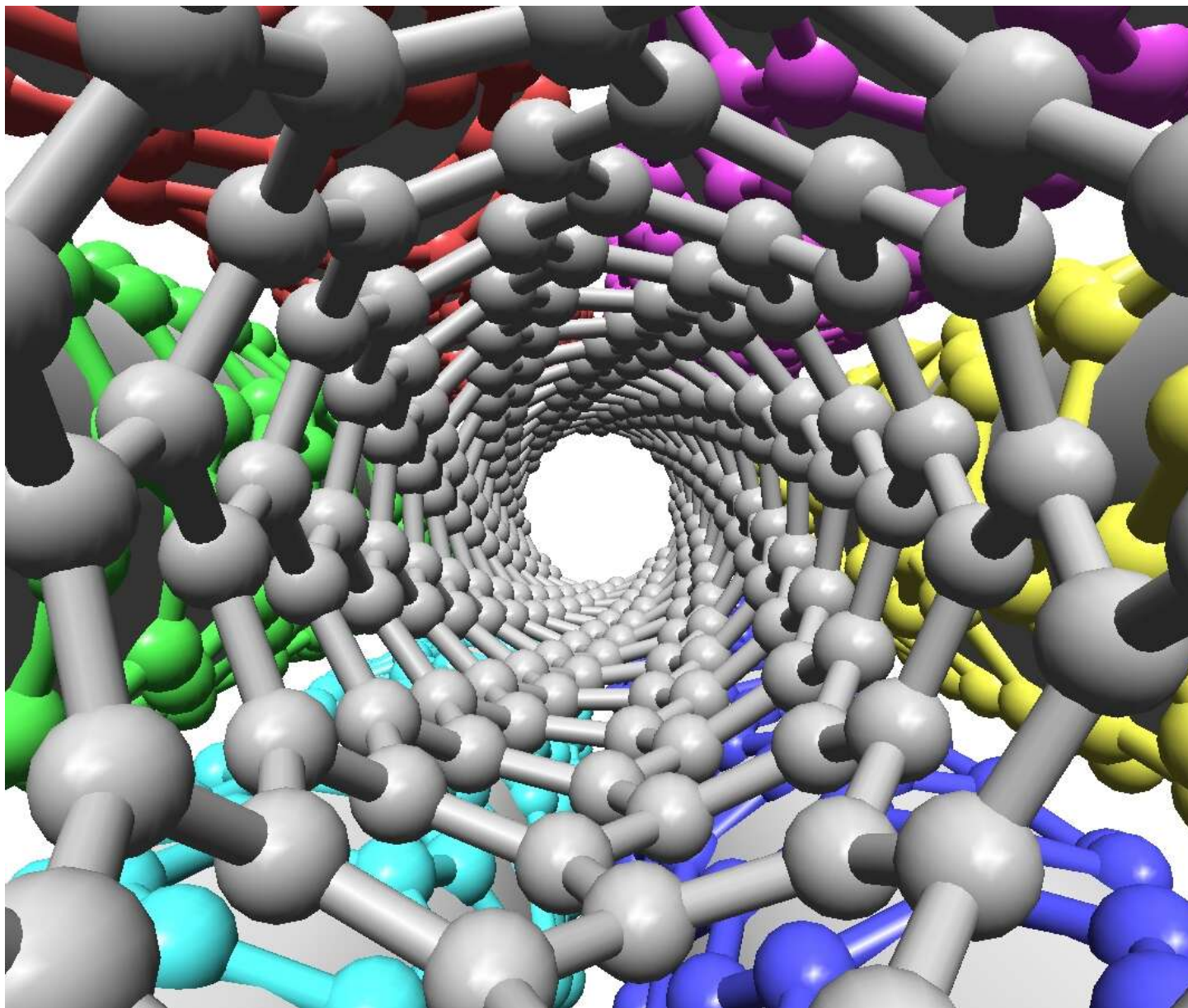
A bundle of seven $\{7,0\}$ single-walled carbon nanotubes (SWCNT)

$\{7,3\}$ Nanotube Bundle



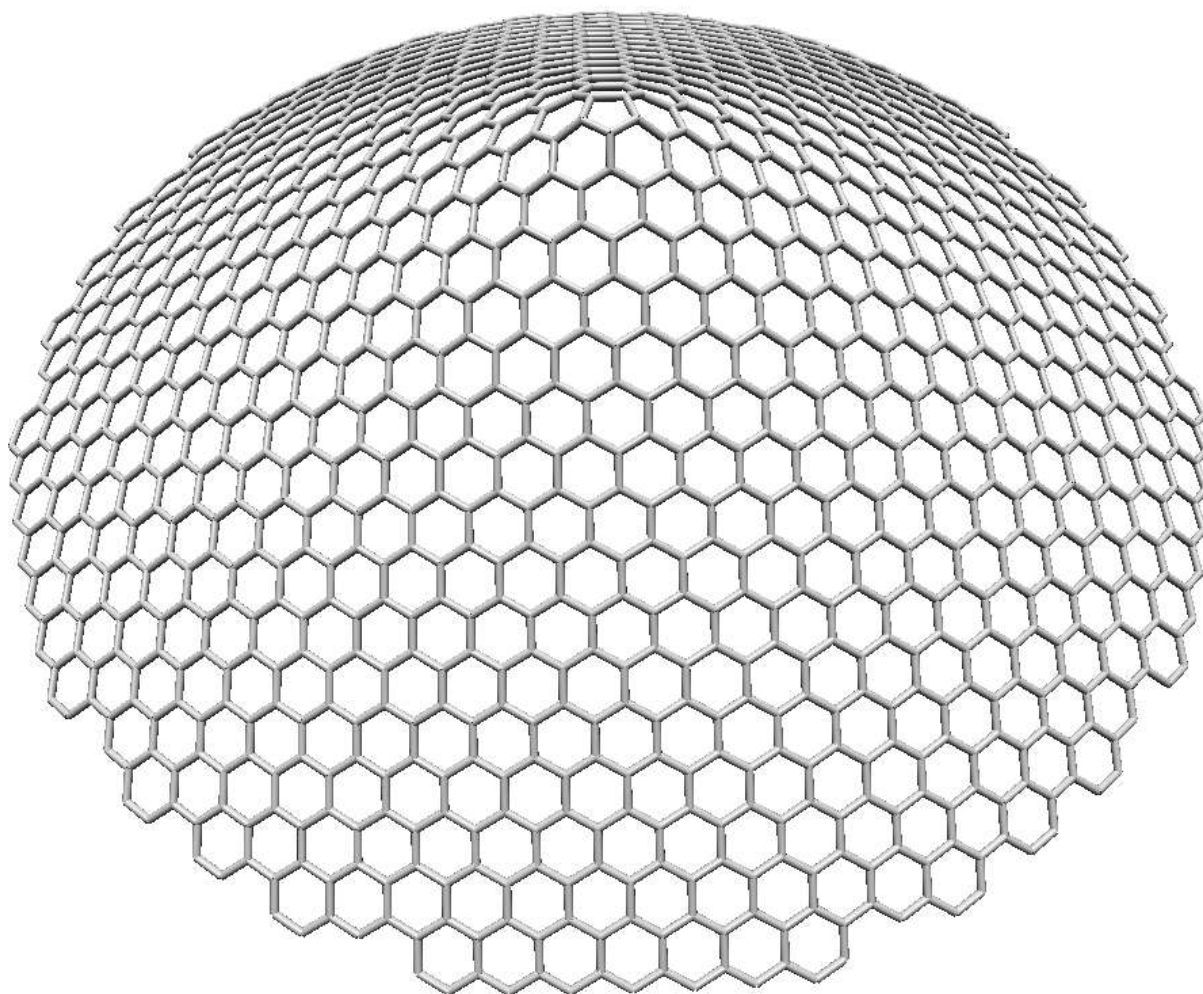
A bundle of seven $\{7,3\}$ nanotubes

Inside {5,3} Nanotube



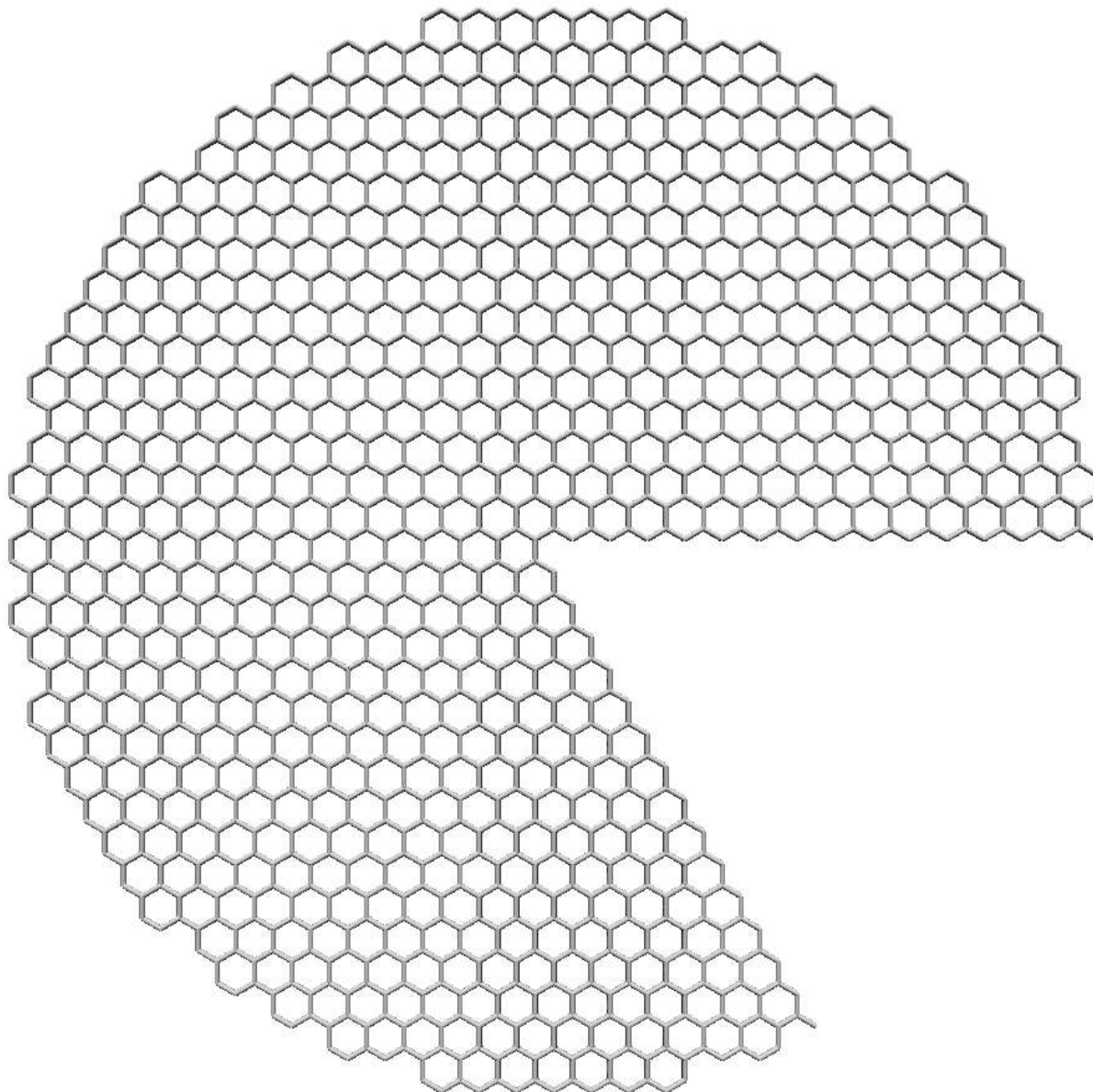
Looking inside a bundle of {5,3} nanotubes

60° - Nanocone



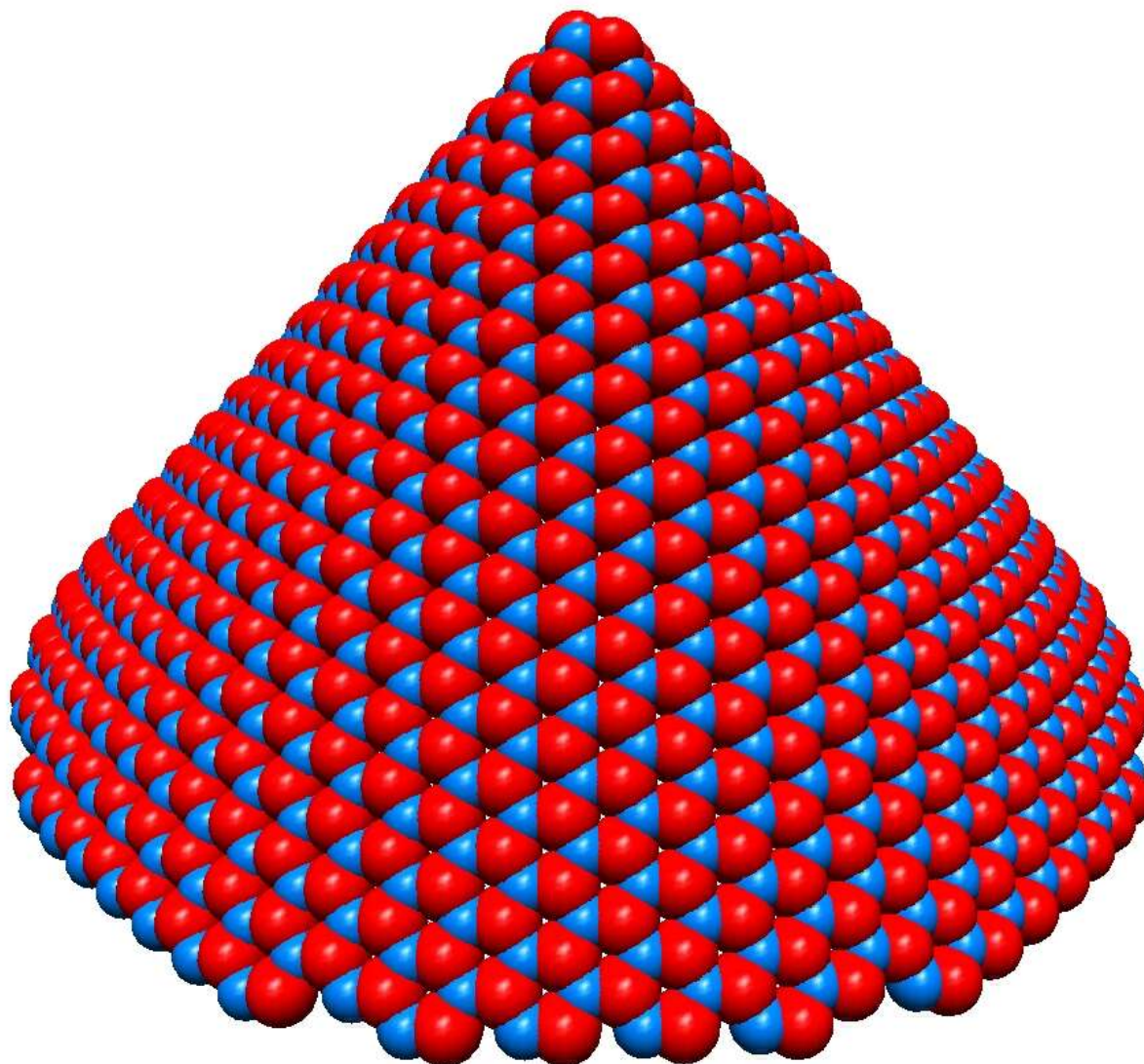
Disclination angle 60°
Cone height 20 Å

60° - Nanocone Sheet



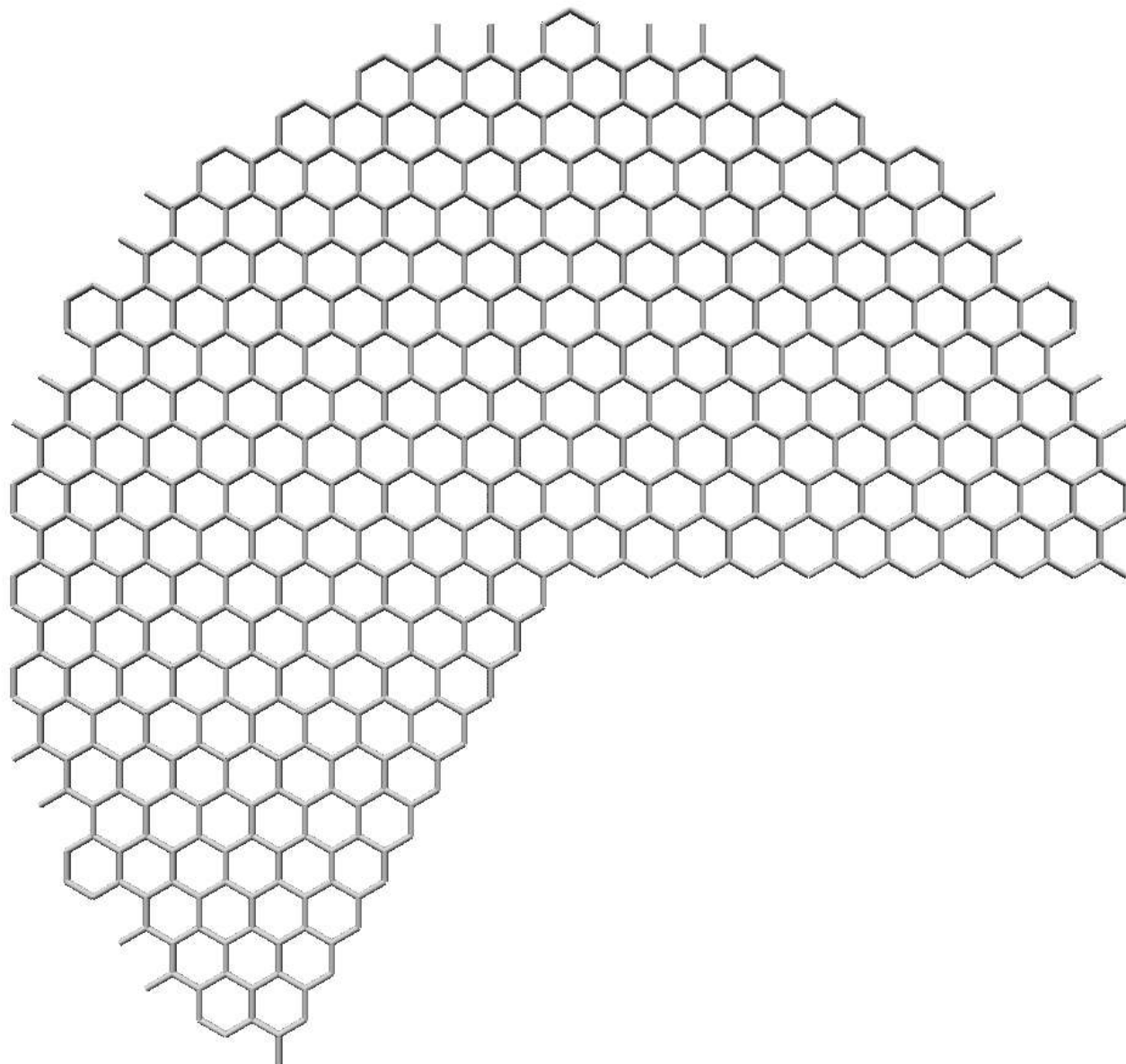
Disclination angle 60°
Creates a cone of height 20 \AA

120° - Nanocone



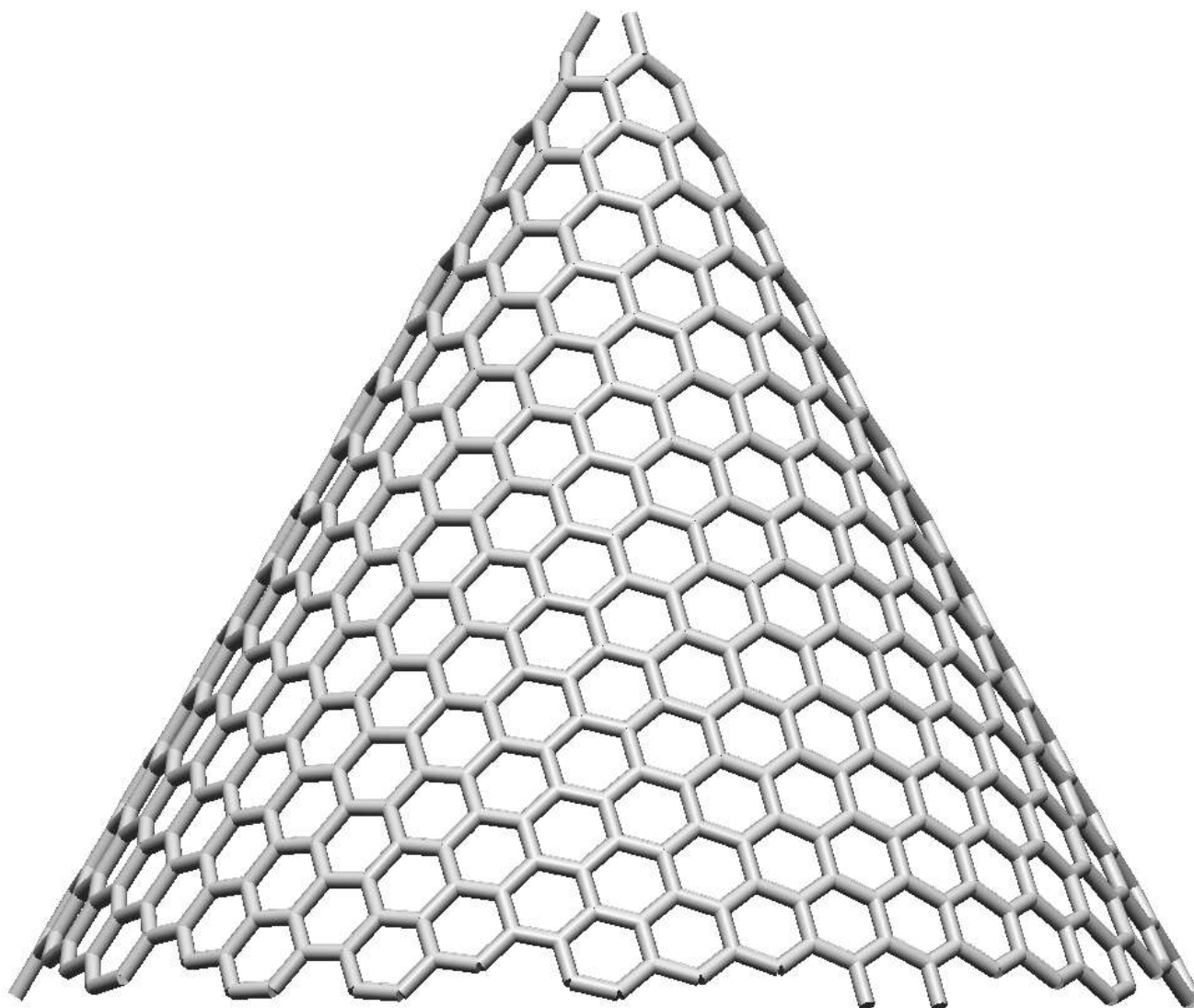
Disclination angle 120°
Cone height 30 \AA

120° - Nanocone Sheet



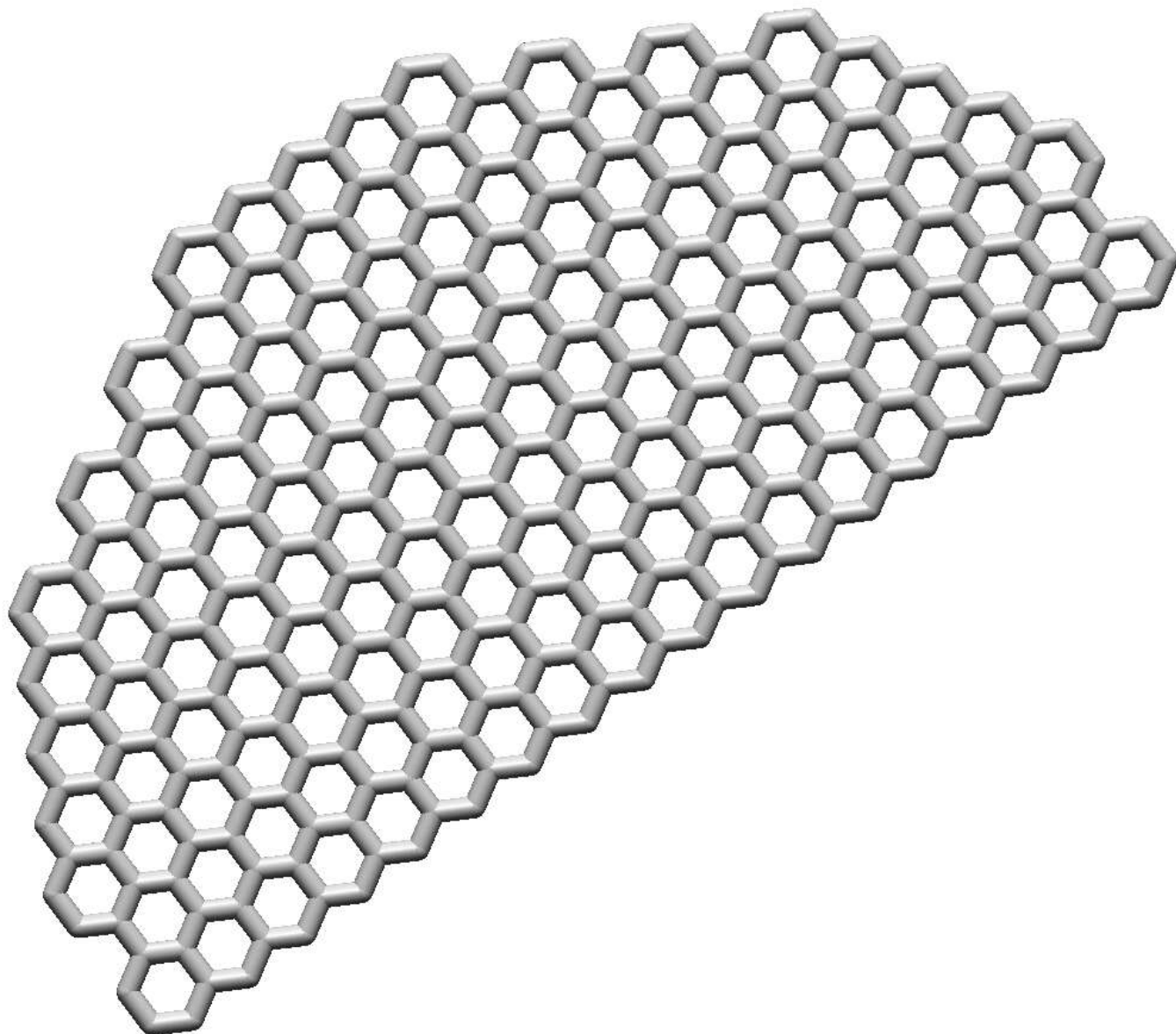
Disclination angle 120°
Creates a cone of height 20 \AA

180° - Nanocone



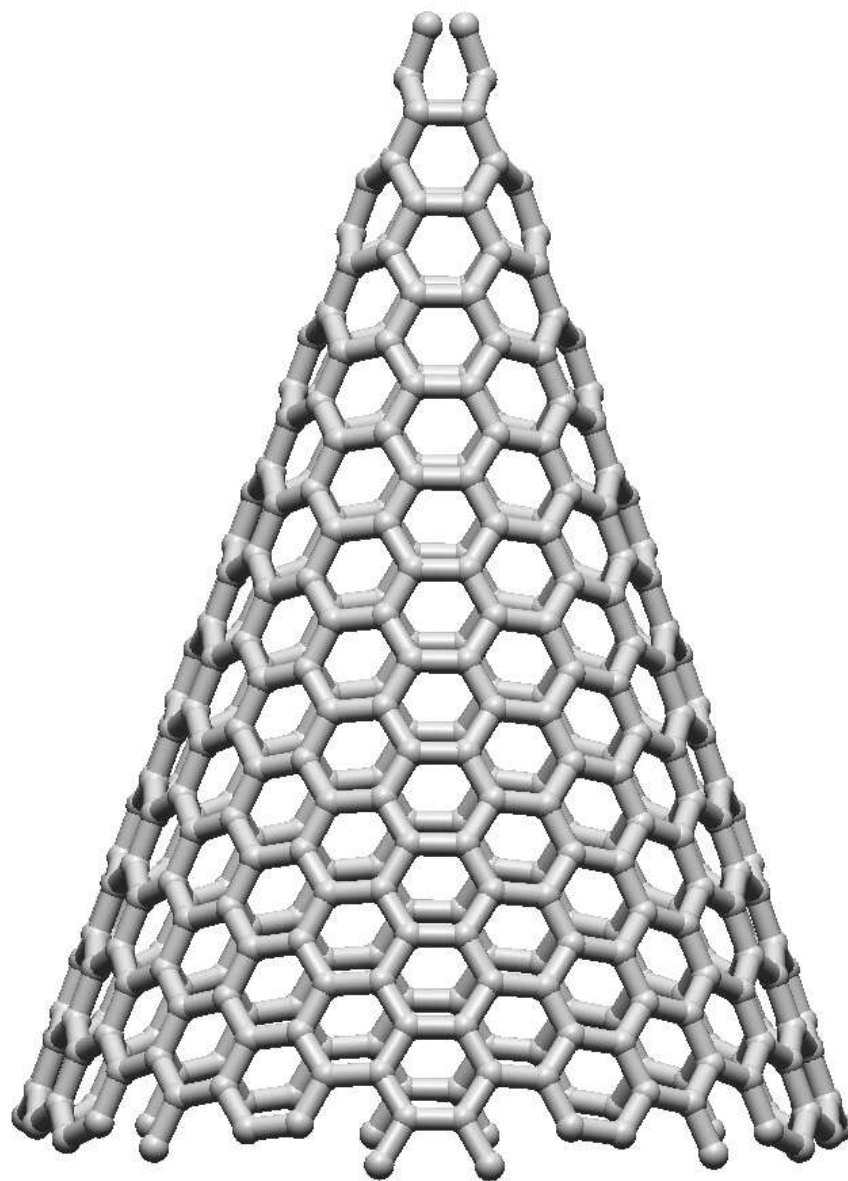
Disclination angle 180°
Cone height 30 \AA

180° - Nanocone Sheet



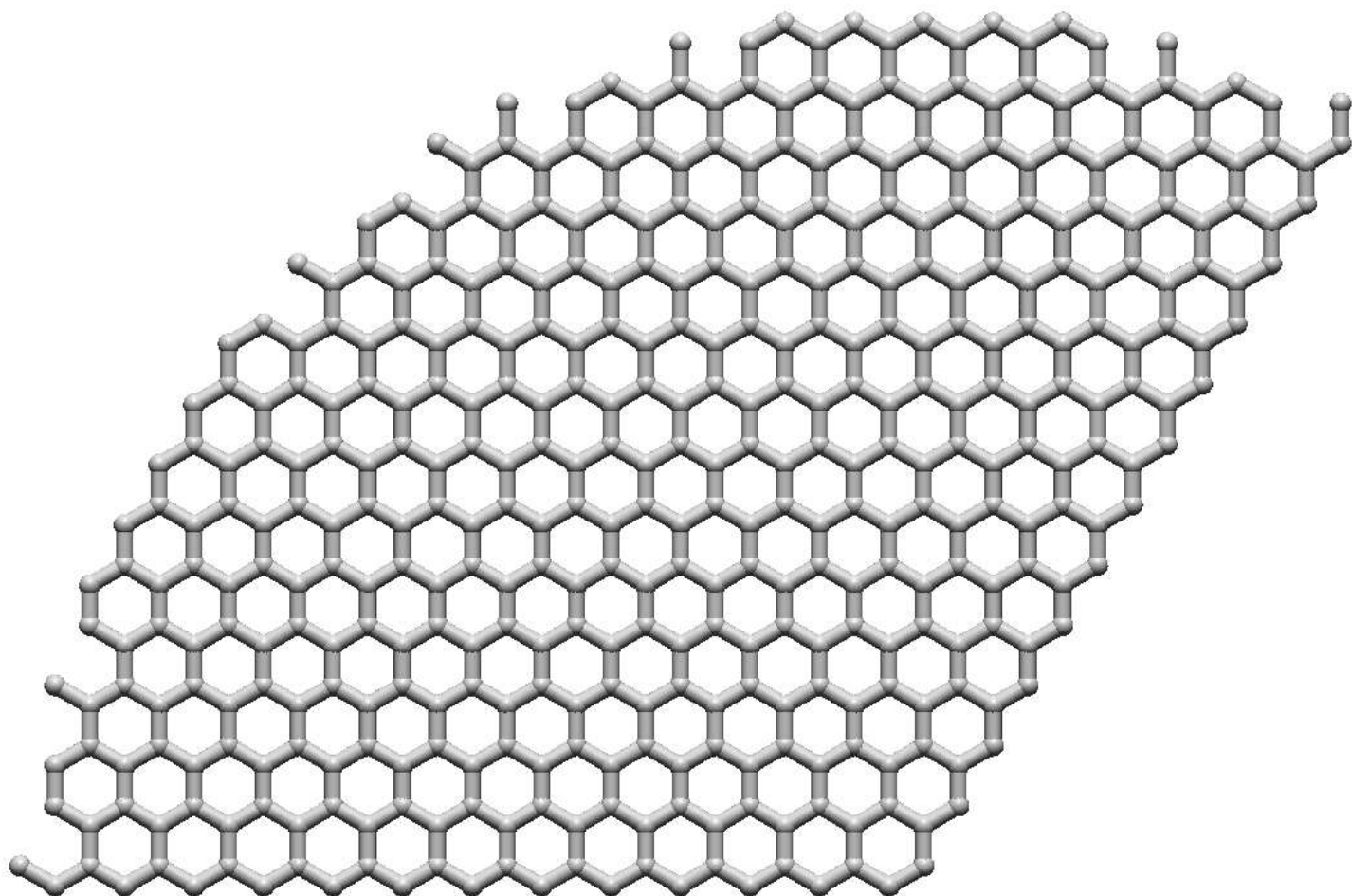
Disclination angle 180°
Creates a cone of height 20 \AA

240° - Nanocone



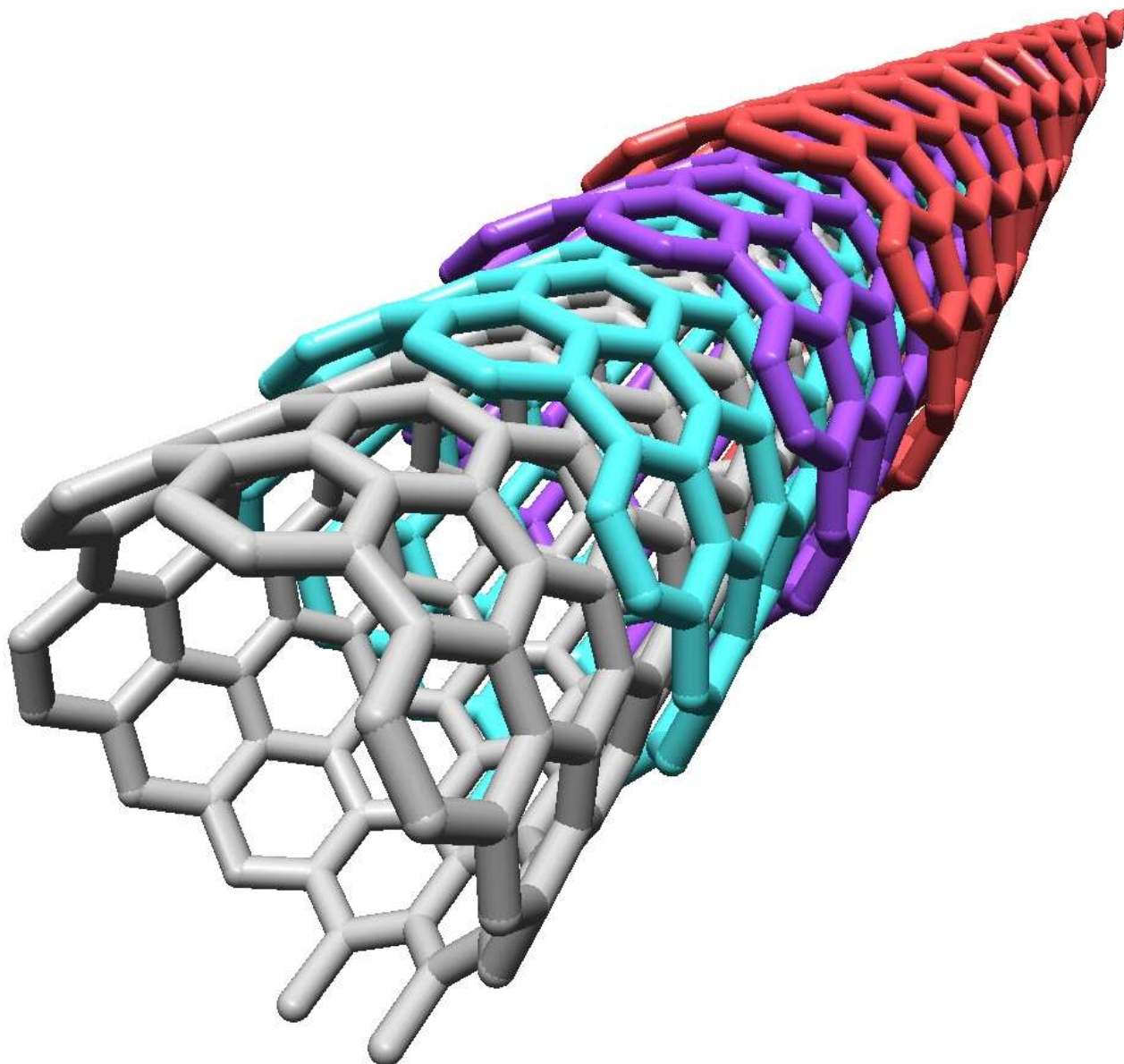
Disclination angle 240°
Cone height 30 \AA

240° - Nanocone Sheet



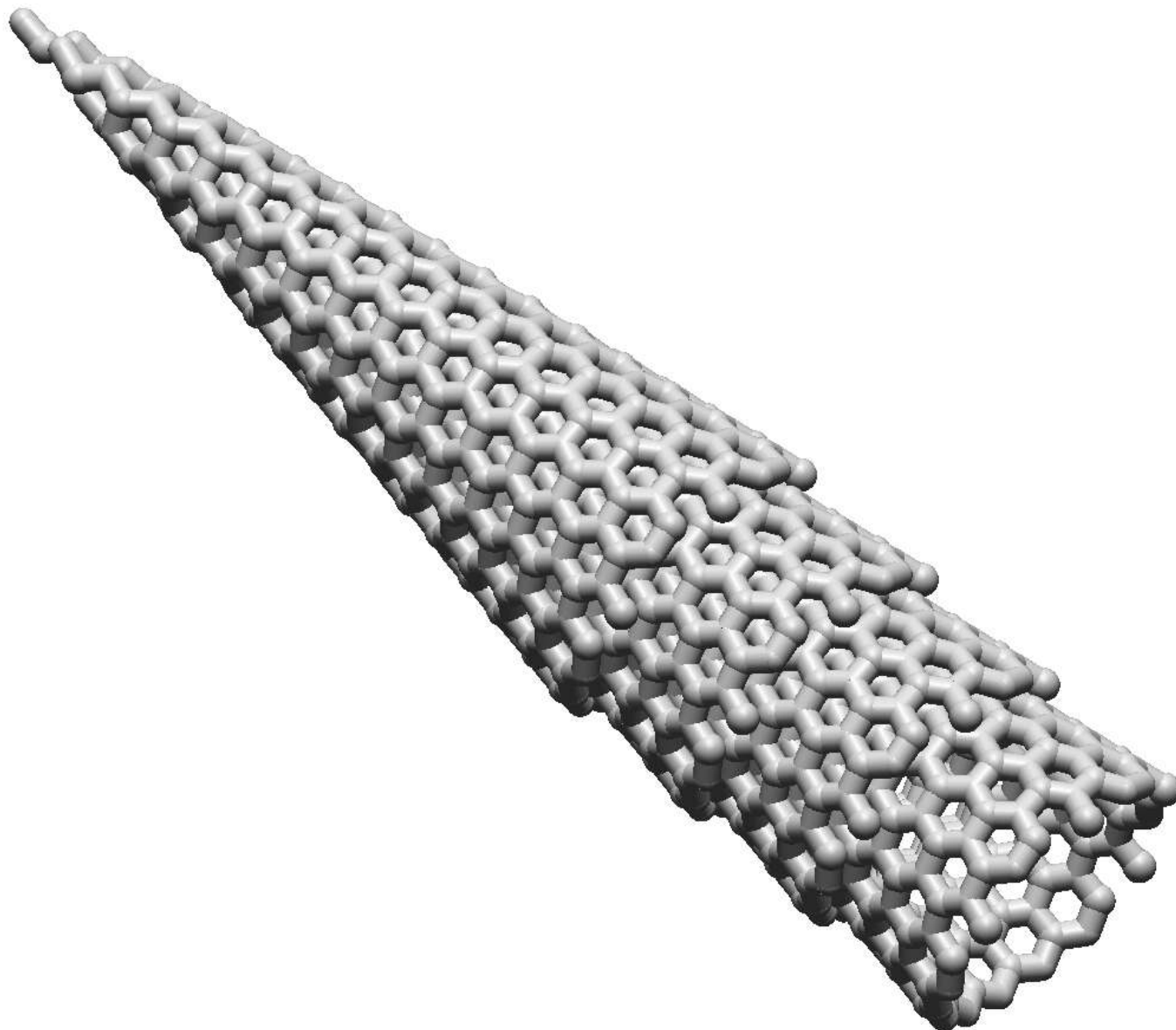
Disclination angle 240°
Creates a cone of height 30 \AA

300° - Nanocone Stack



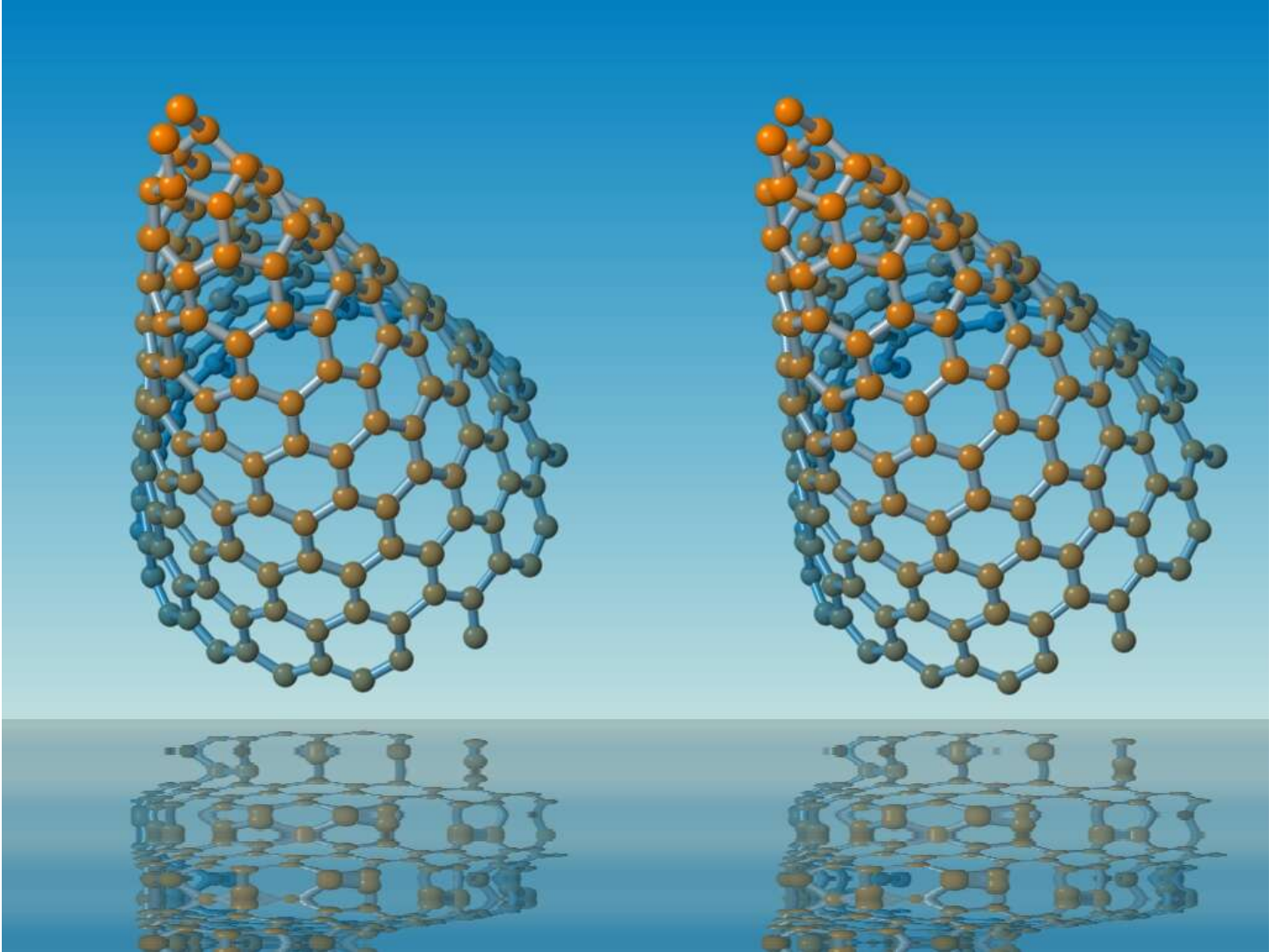
Disclination angle 300°
Four cones of height 30 \AA

300° - Nanocone Stack



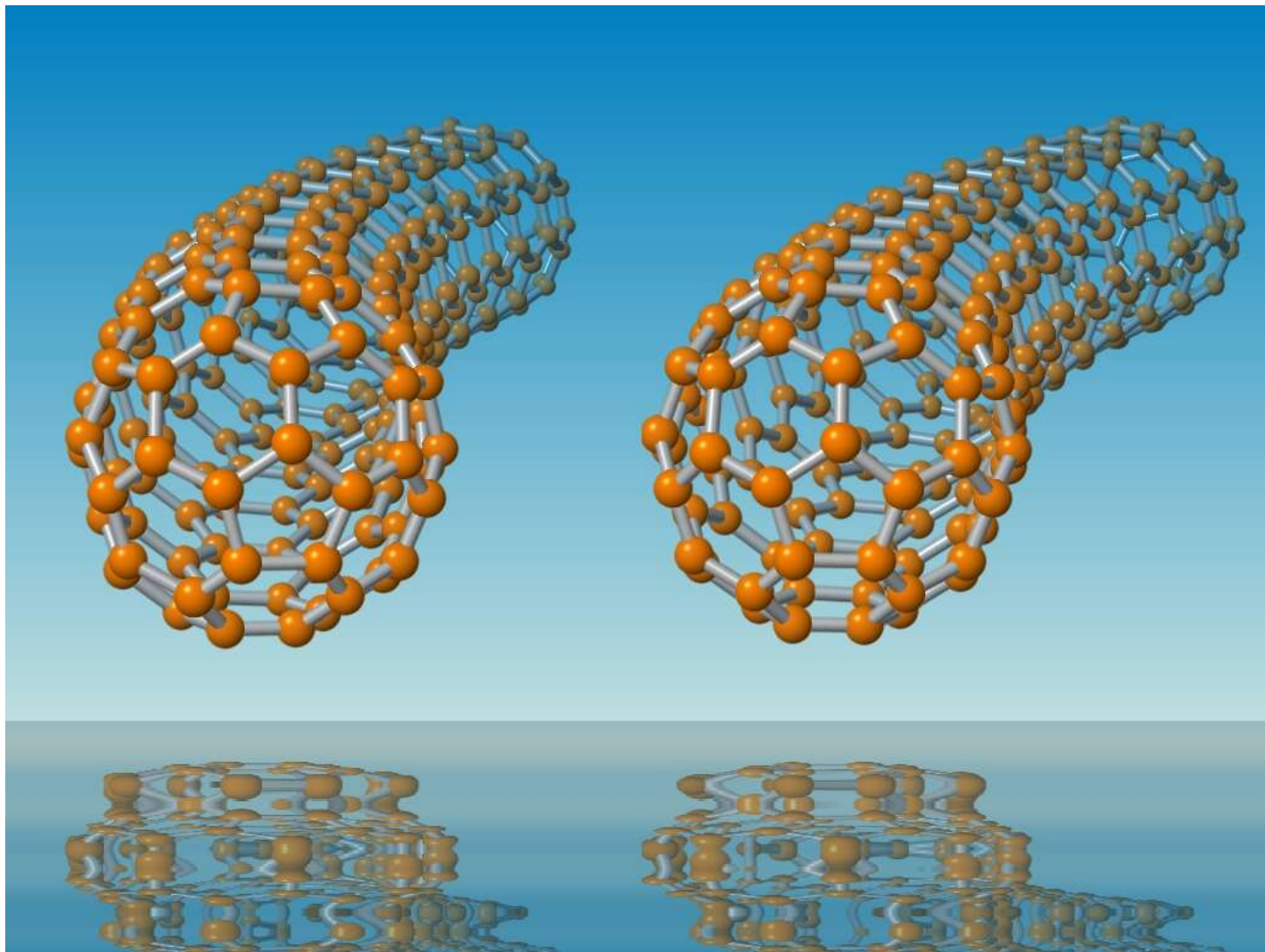
Disclination angle 300°
Four cones of height 40 \AA

Nanocone Stereo Pair



Disclination angle 240° , Cone height 20 Å, Stereo view (relaxed-eye view)
This image was created with JPOWD from MDI (www.materialsdata.com)

Nanotube Stereo Pair



A bent capped {5,5} nanotube in stereo view (relaxed-eye view).
This image was created with JPOWD from MDI (www.materialsdata.com)

Disclaimer

I have tried to implement the geometry-generating routines to the best of my knowledge. However, errors in my computer programs may sometimes occur. If you think you found an error please let me know so I can fix it. Please feel free to contact me with suggestions for improvements and additions to these picture books.

You may contact me via email at: *steffenweber@comcast.net*

You may also visit some older galleries of mine at:
jcrystal.com/steffenweber/gallery/NanoTubes/NanoTubes.html
jcrystal.com/steffenweber/gallery/NanoTubes/NanoCones.html

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