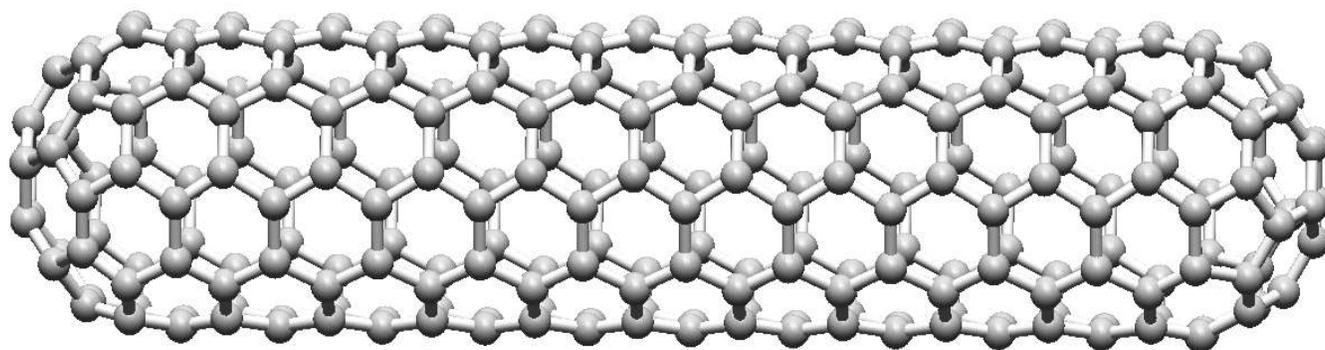


Steffen Weber's

# Crystallography Picture Book

*Nanotubes & Nanocones*



# *Preface*

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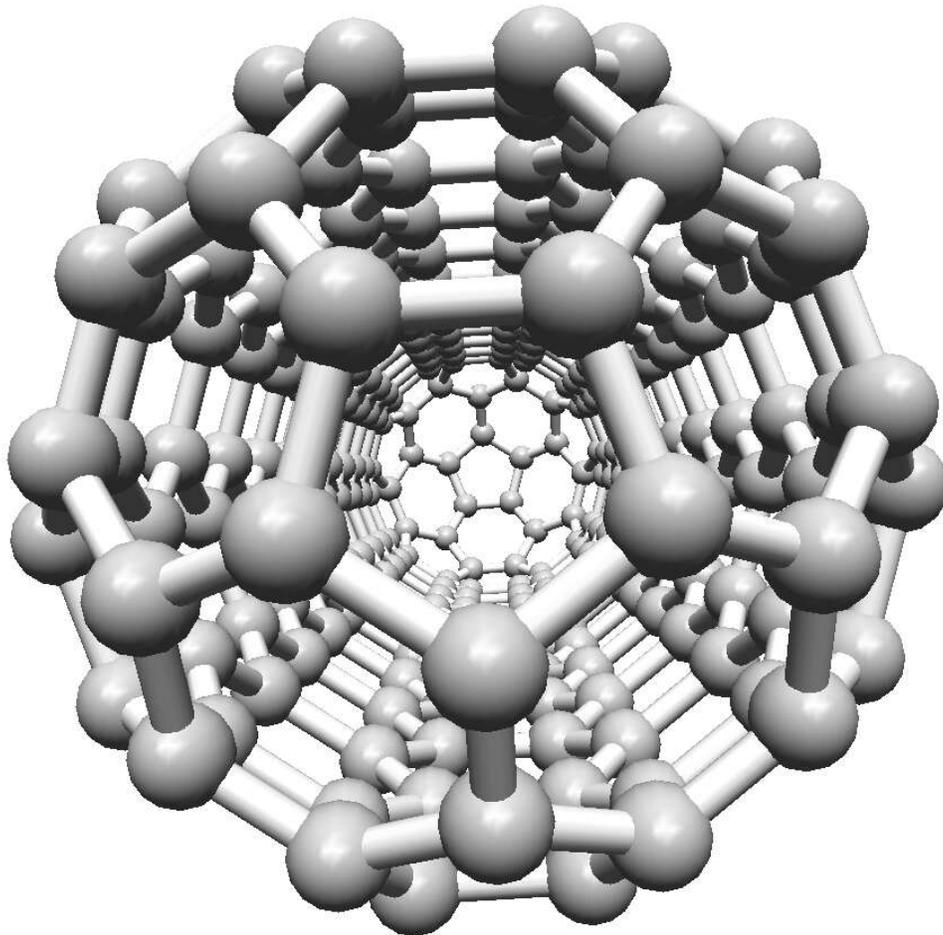
This is the first in a series of picture books that I plan to create for educational purposes. All images in this volume were created using the program *NanotubeModeler* from JCrystalSoft. A free version of this program can be downloaded at [www.jcrystal.com](http://www.jcrystal.com). My earliest implementation 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](http://www.jcrystal.com/steffenweber)

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# *Capped {5,5} Tube*

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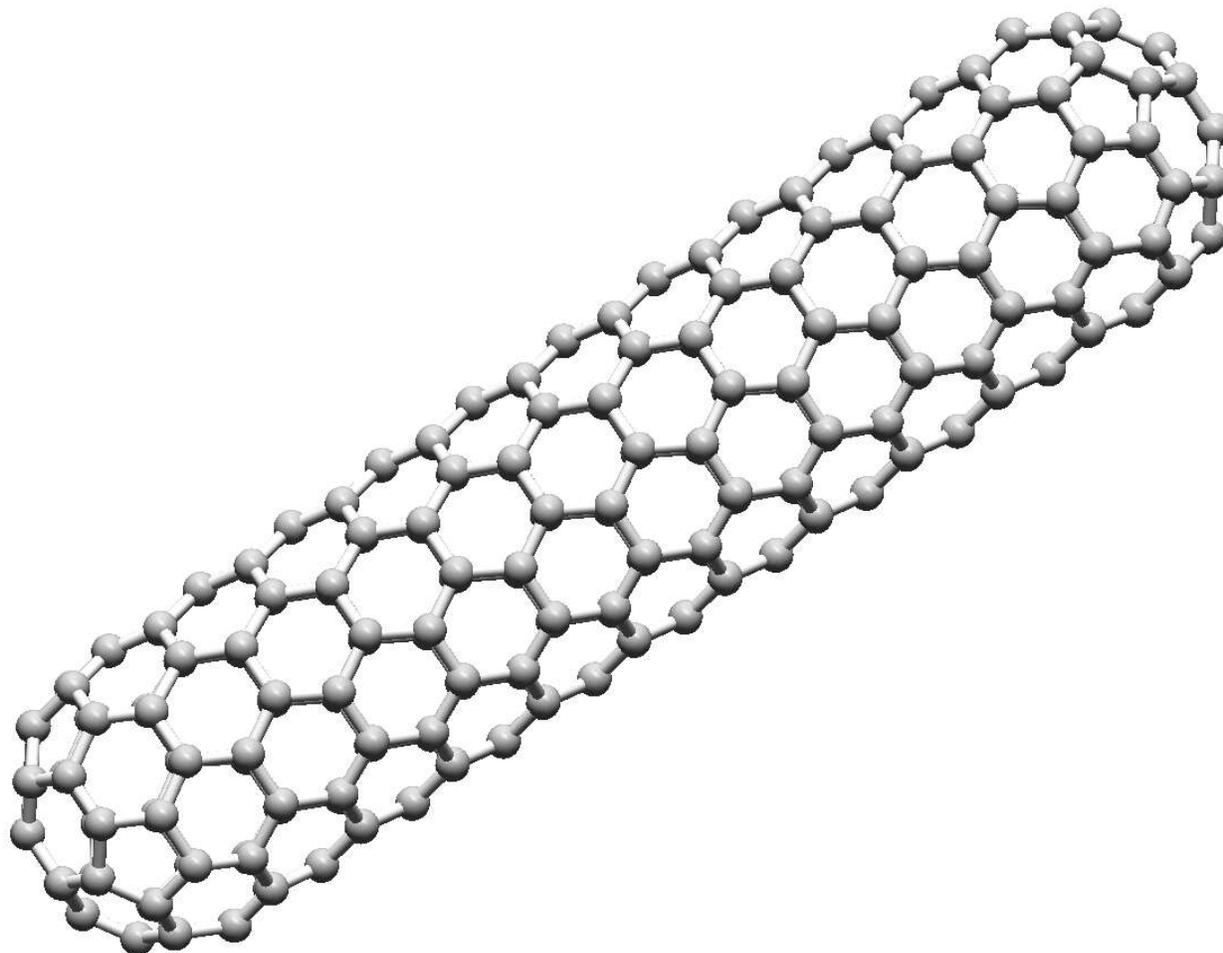


Carbon Nanotube  
Armchair structure with Bucky-ball caps

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# *Capped {5,5} Tube*

---

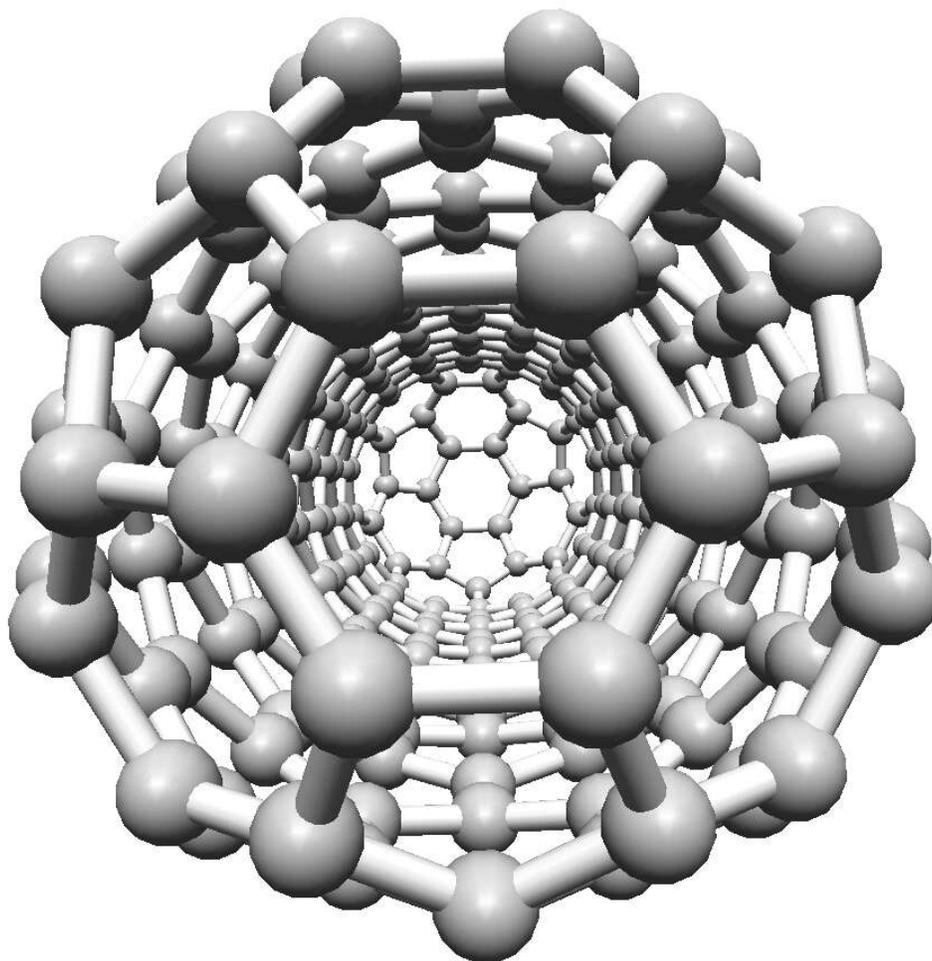


Carbon Nanotube  
Armchair structure with Bucky-ball caps  
Length  $\sim 25$  Å, Diameter  $\sim 6.75$  Å

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# *Capped {9,0} Tube*

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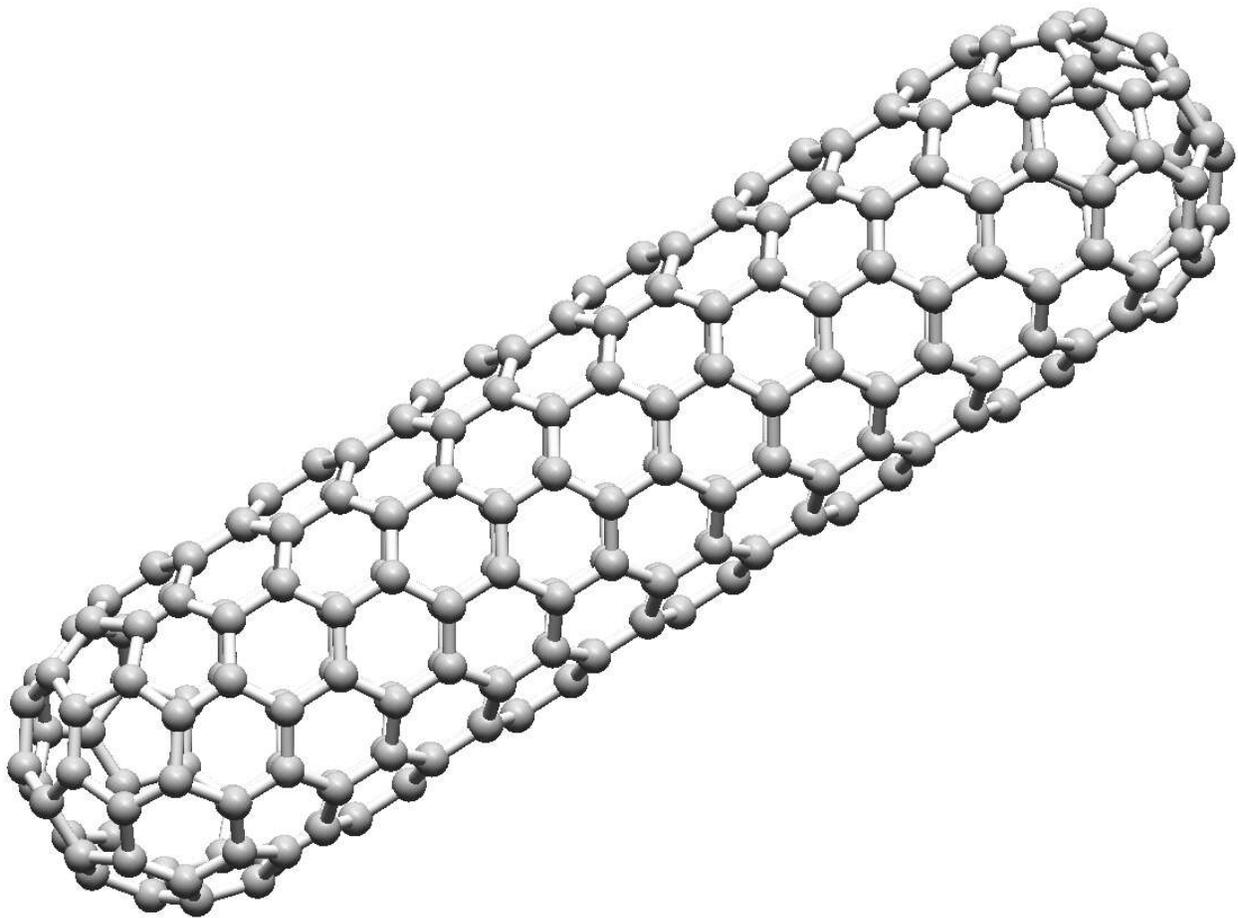


Carbon Nanotube  
Zigzag structure with Bucky-ball caps

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# *Capped {9,0} Tube*

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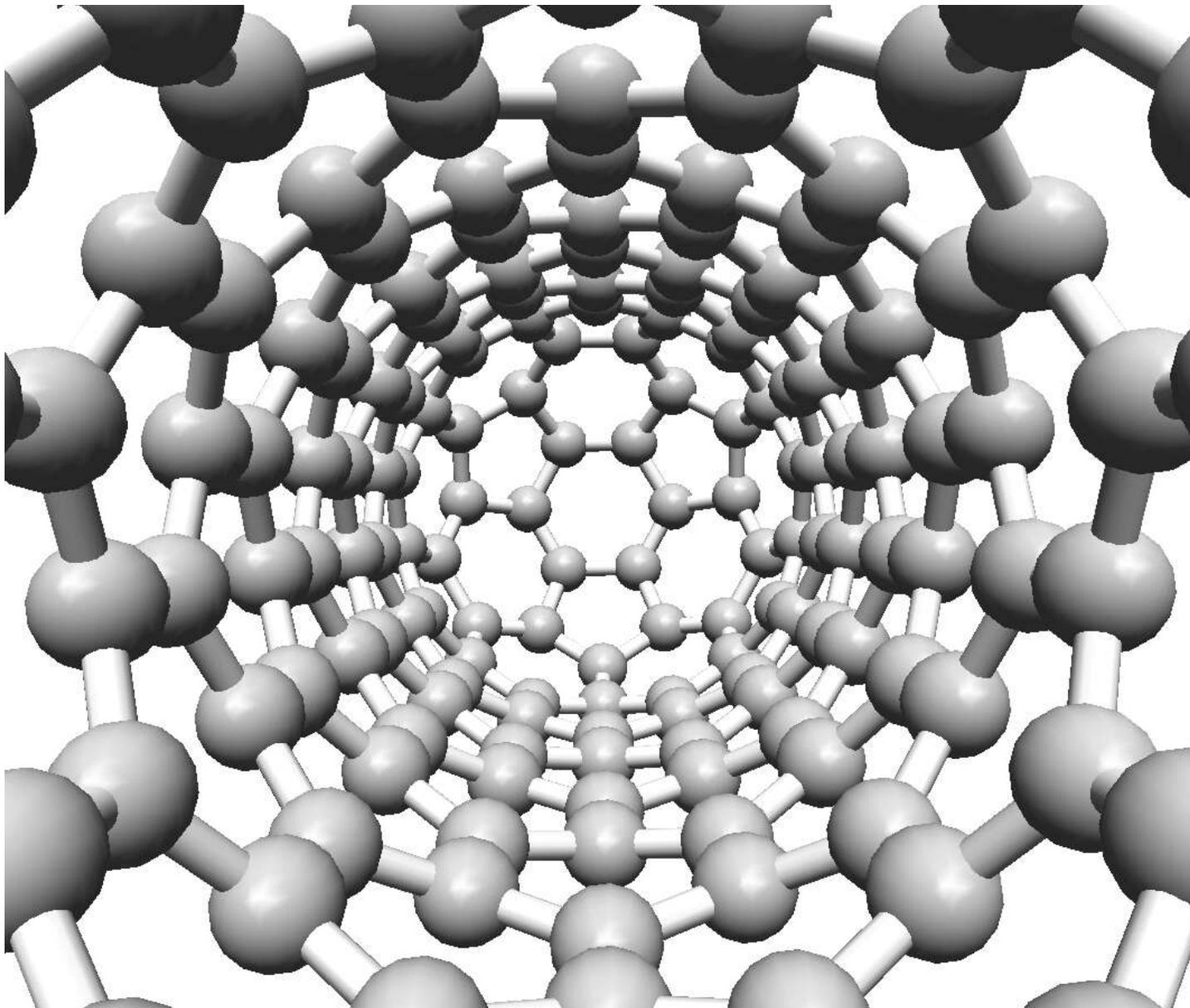


Carbon Nanotube  
Armchair structure with Bucky-ball caps  
Length  $\sim 25 \text{ \AA}$ , Diameter  $\sim 6.99 \text{ \AA}$

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# *Inside Capped {9,0} Tube*

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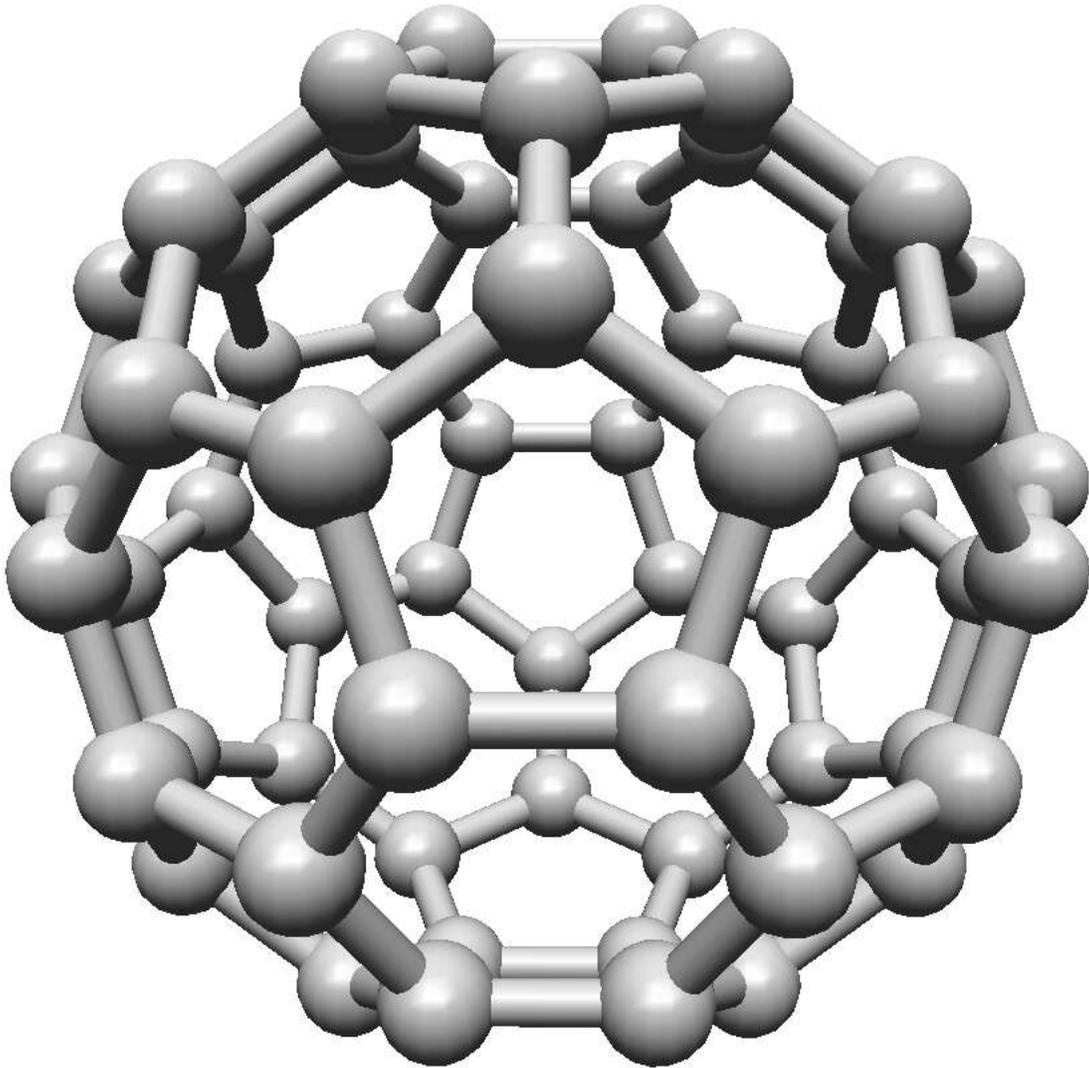


Inside a capped {9,0} nanotube

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# *Bucky-Ball ( $C_{60}$ )*

---

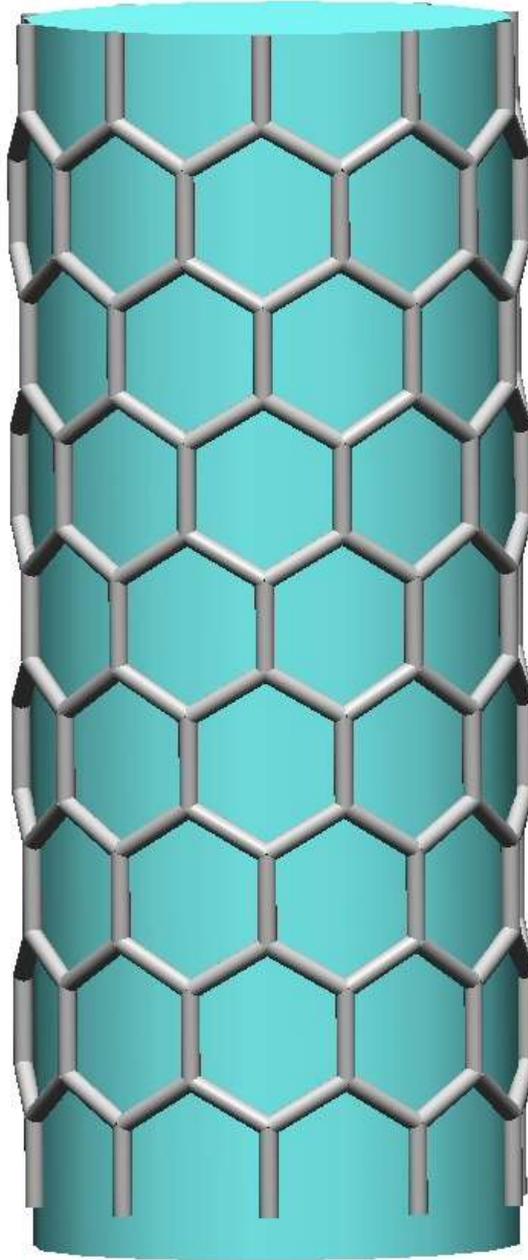


A Buckyball, the well-known Fullerene with icosahedral symmetry. Two different sections of the Buckyball can be used to cap the {5,5} and {9,0} nanotubes.

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# *$\{10,0\}$ Nanotube*

---

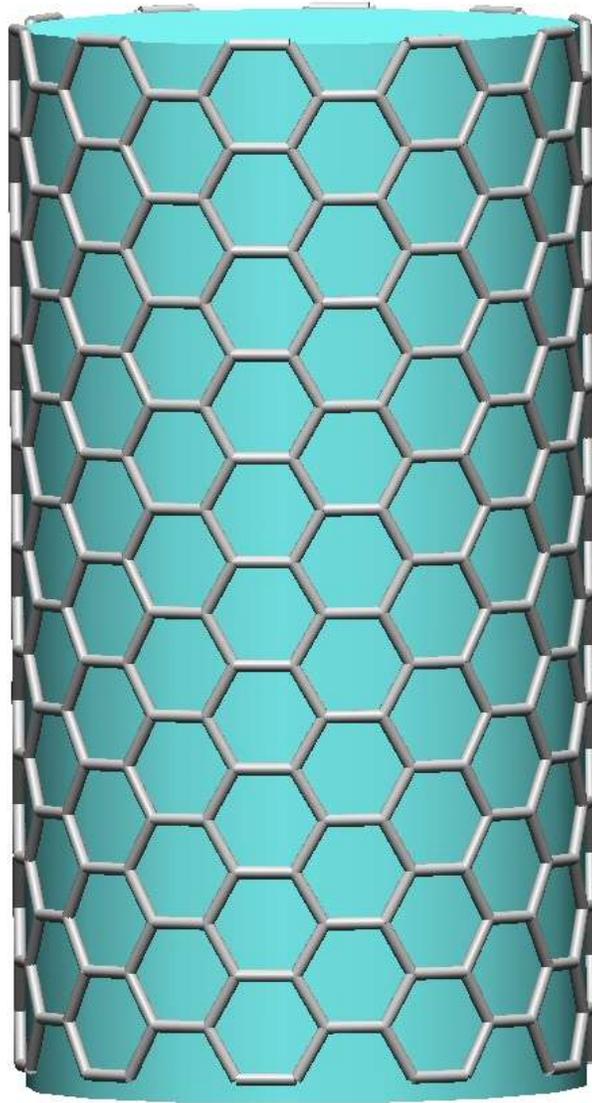


Zig-zag structure  
Length  $\sim 19$  Å, Diameter  $\sim 7.77$  Å

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# *$\{10,10\}$ Nanotube*

---

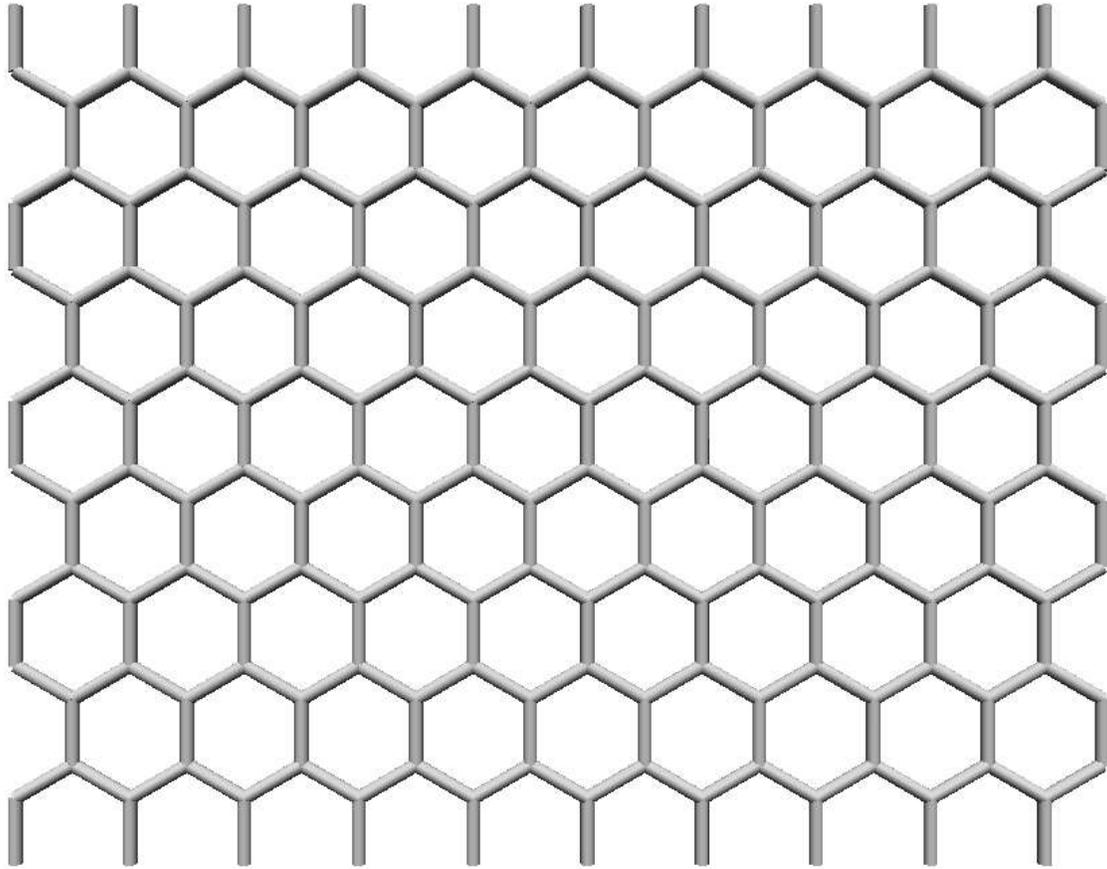


Armchair structure  
Length  $\sim 25 \text{ \AA}$ , Diameter  $\sim 13.465 \text{ \AA}$

---

# *$\{10,0\}$ Graphene Sheet*

---

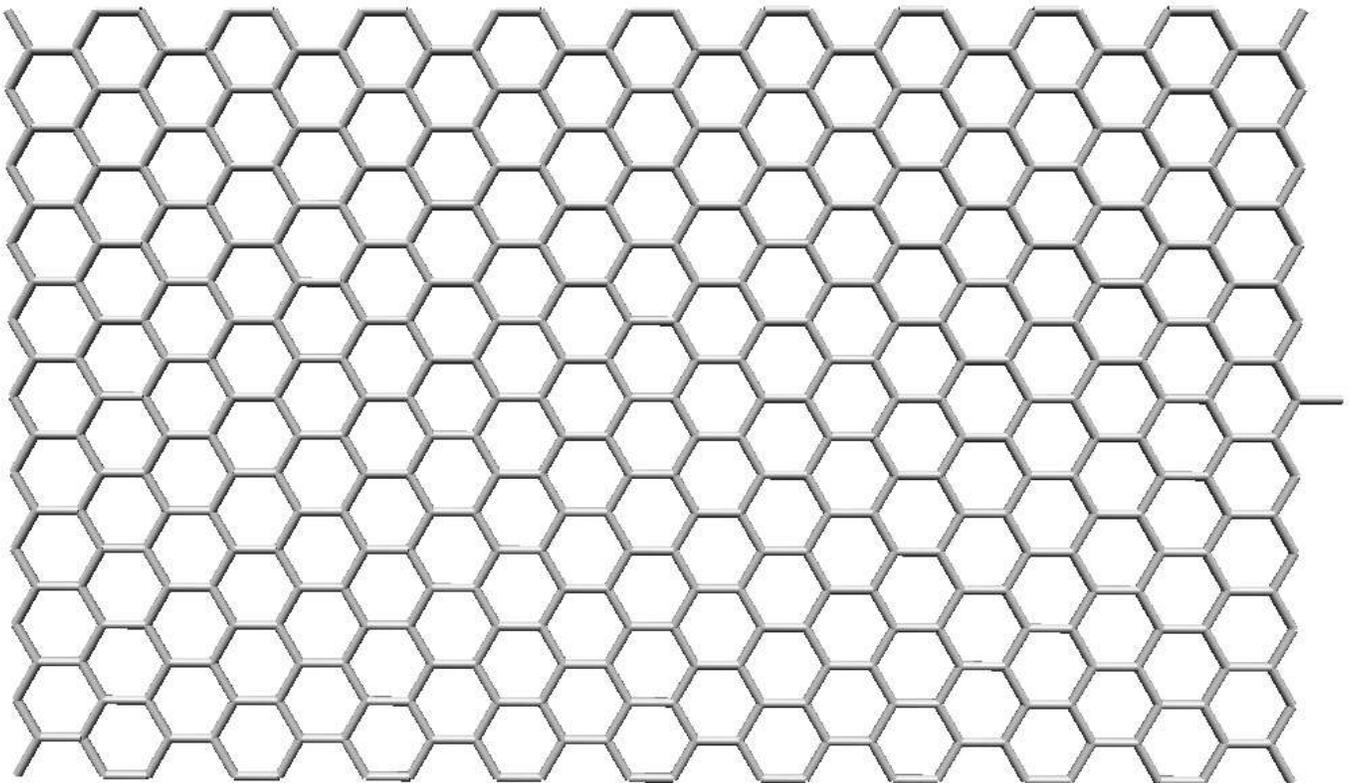


Zig-zag structure  
This sheet can be rolled into a  $\{10,0\}$  nanotube

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# ***{10,10} Graphene Sheet***

---

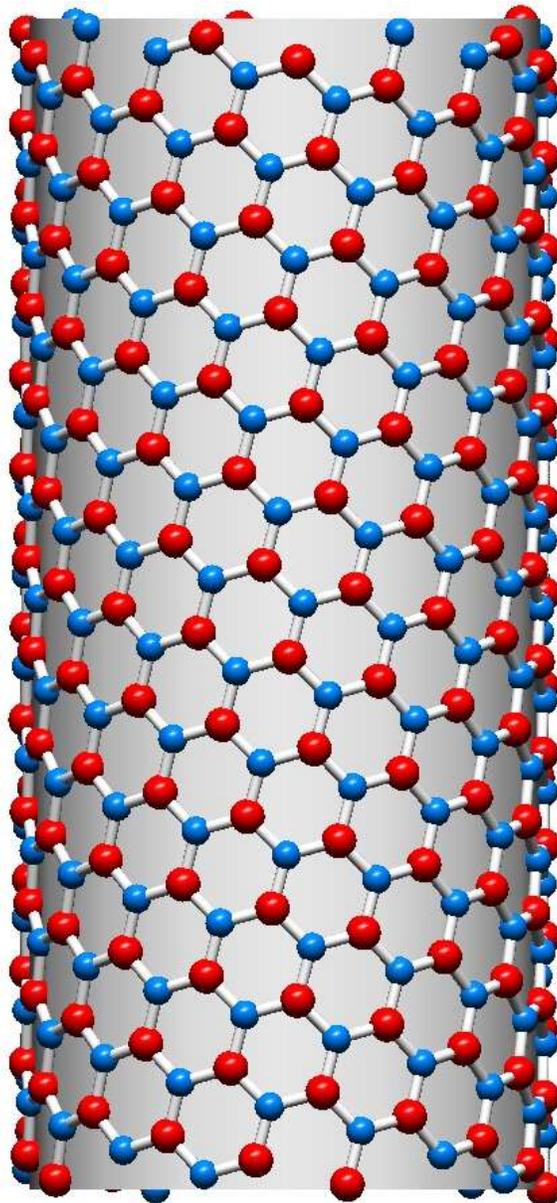


Armchair structure  
This sheet can be rolled into a {10,10} nanotube

---

# *$\{14,5\}$ BN-Nanotube*

---

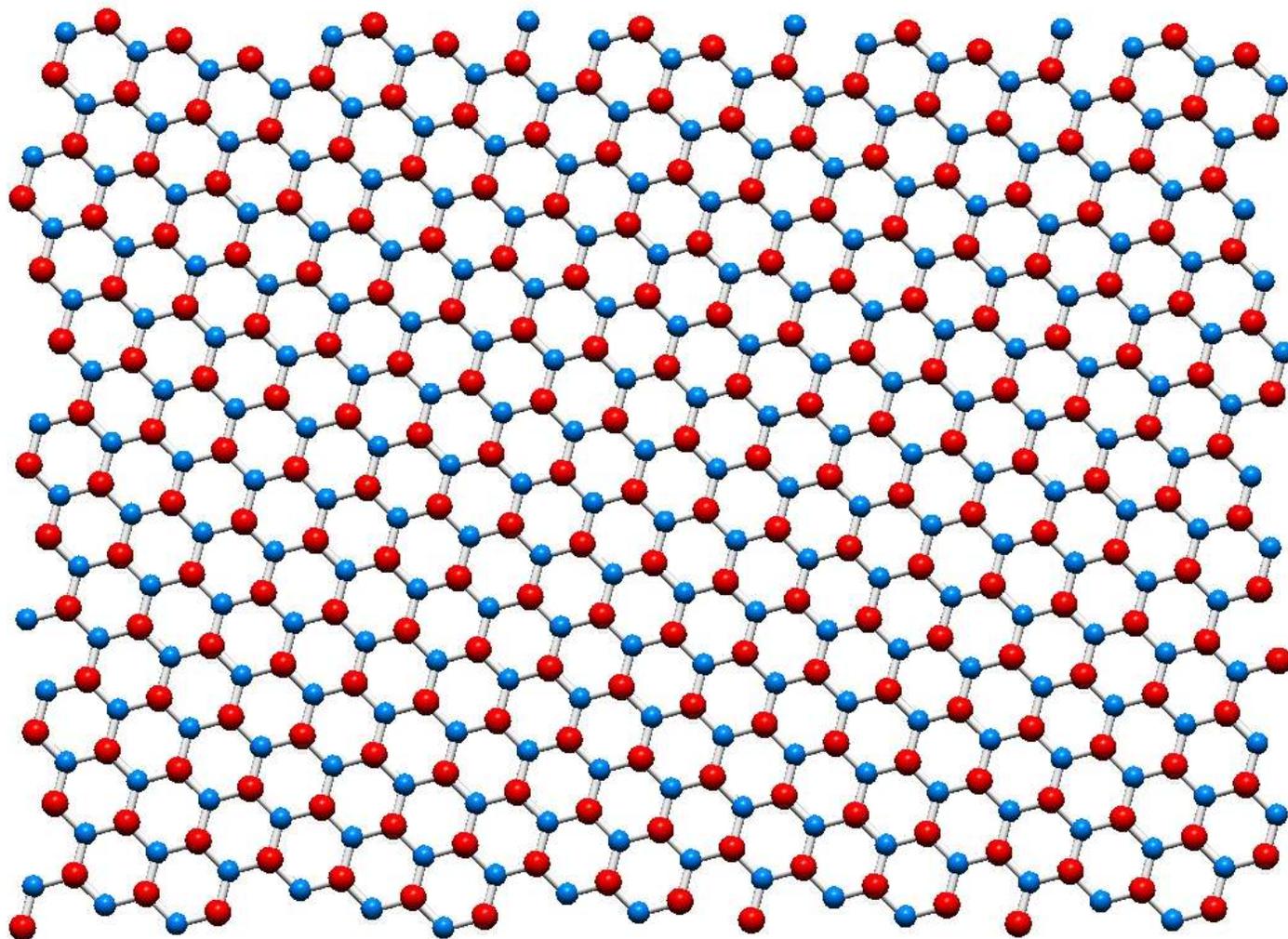


Chiral Boron-Nitride nanotube  
Length  $\sim 30 \text{ \AA}$ , Diameter  $\sim 13.26 \text{ \AA}$

---

# *$\{14,5\}$ BN-Sheet*

---

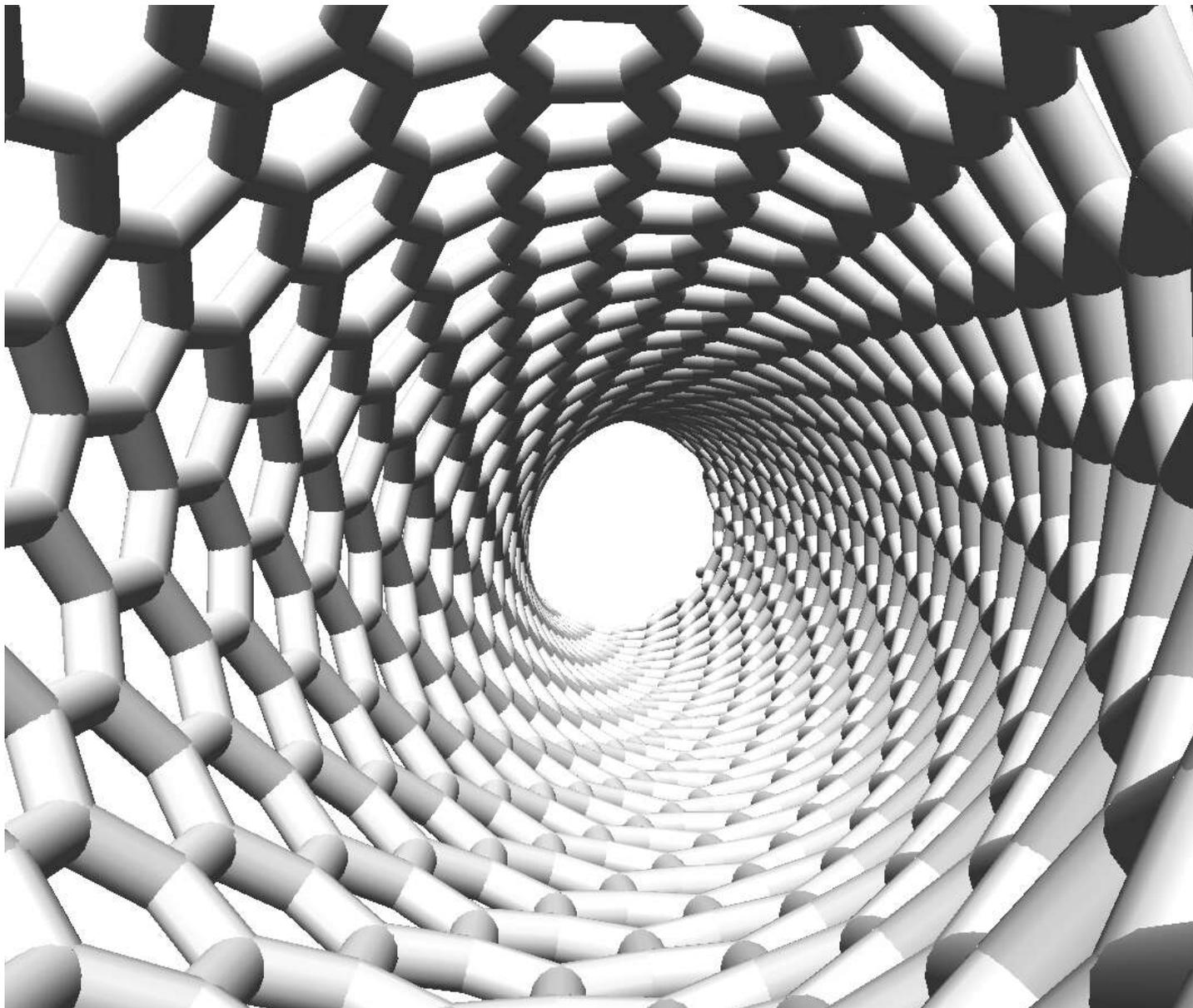


Chiral structure  
This sheet can be rolled into a  $\{14,5\}$  nanotube

---

# *Inside {14,5} Nanotube*

---

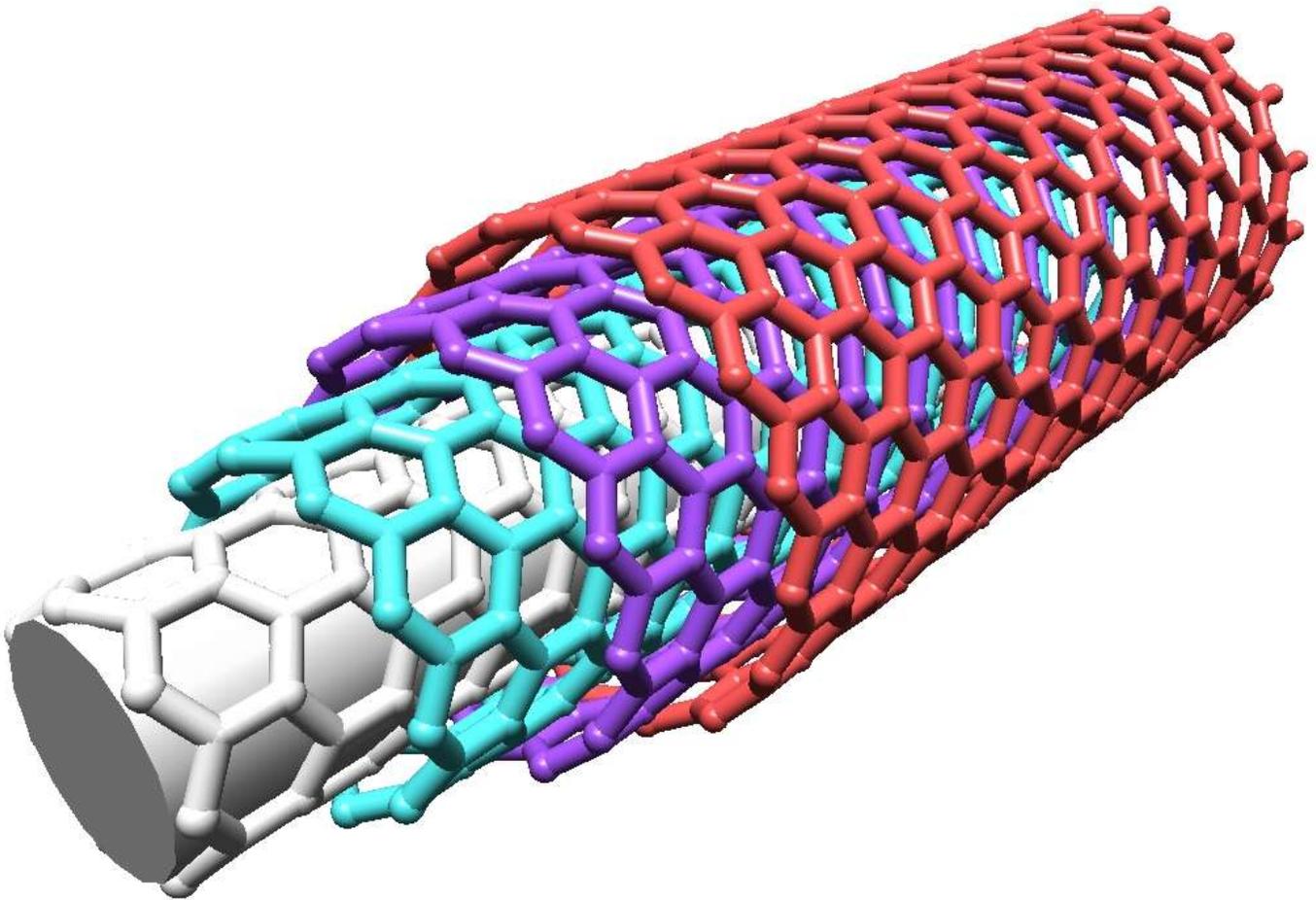


Inside a bent {14,5} nanotube

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# *MWCNT*

---

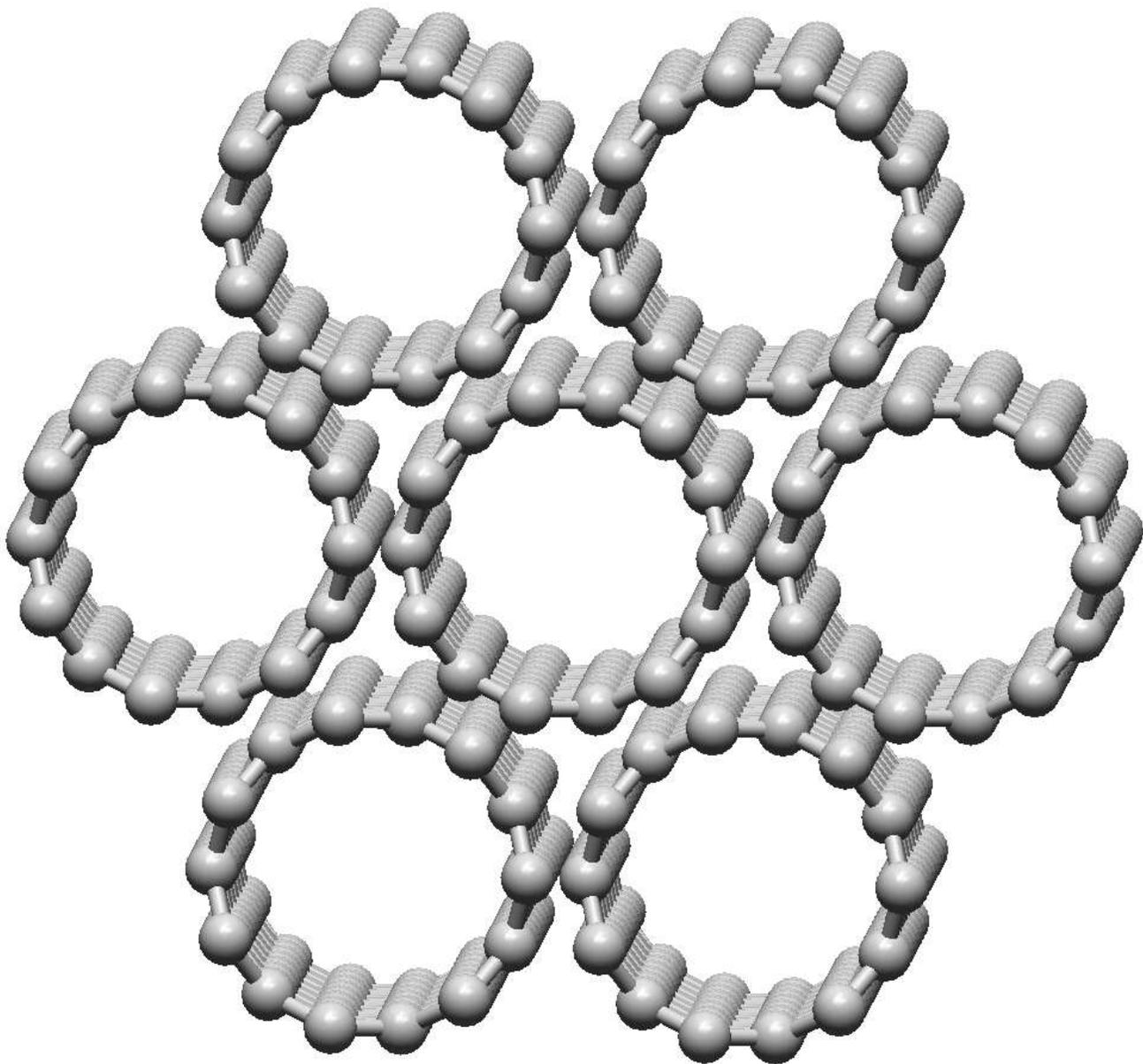


A multi-walled carbon nanotube (MWCNT)  
{7,0}, {10,0}, {13,0} and {16,0} tubes

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# *$\{7,0\}$ Nanotube Bundle*

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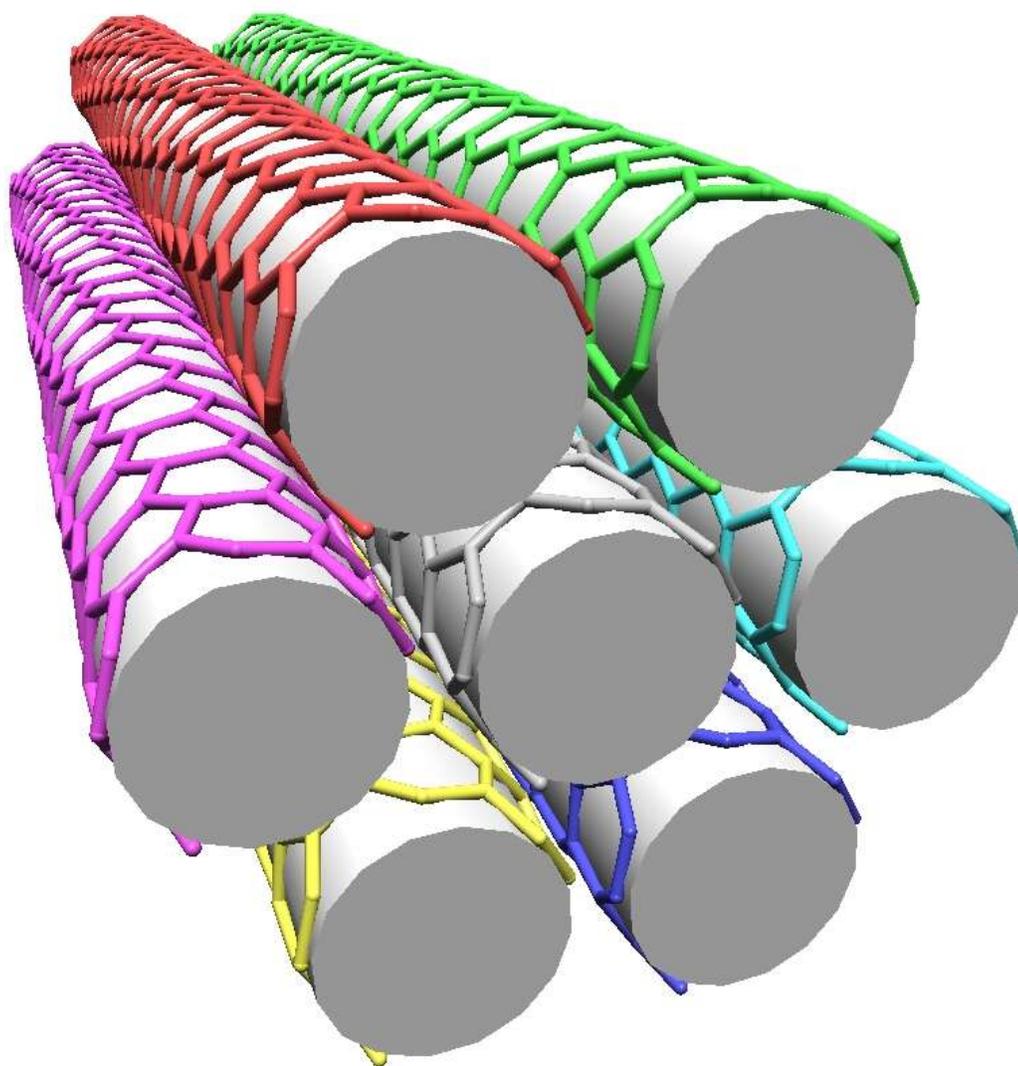


A bundle of seven  $\{7,0\}$  single-walled carbon nanotubes (SWCNT)

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# *$\{7,3\}$ Nanotube Bundle*

---

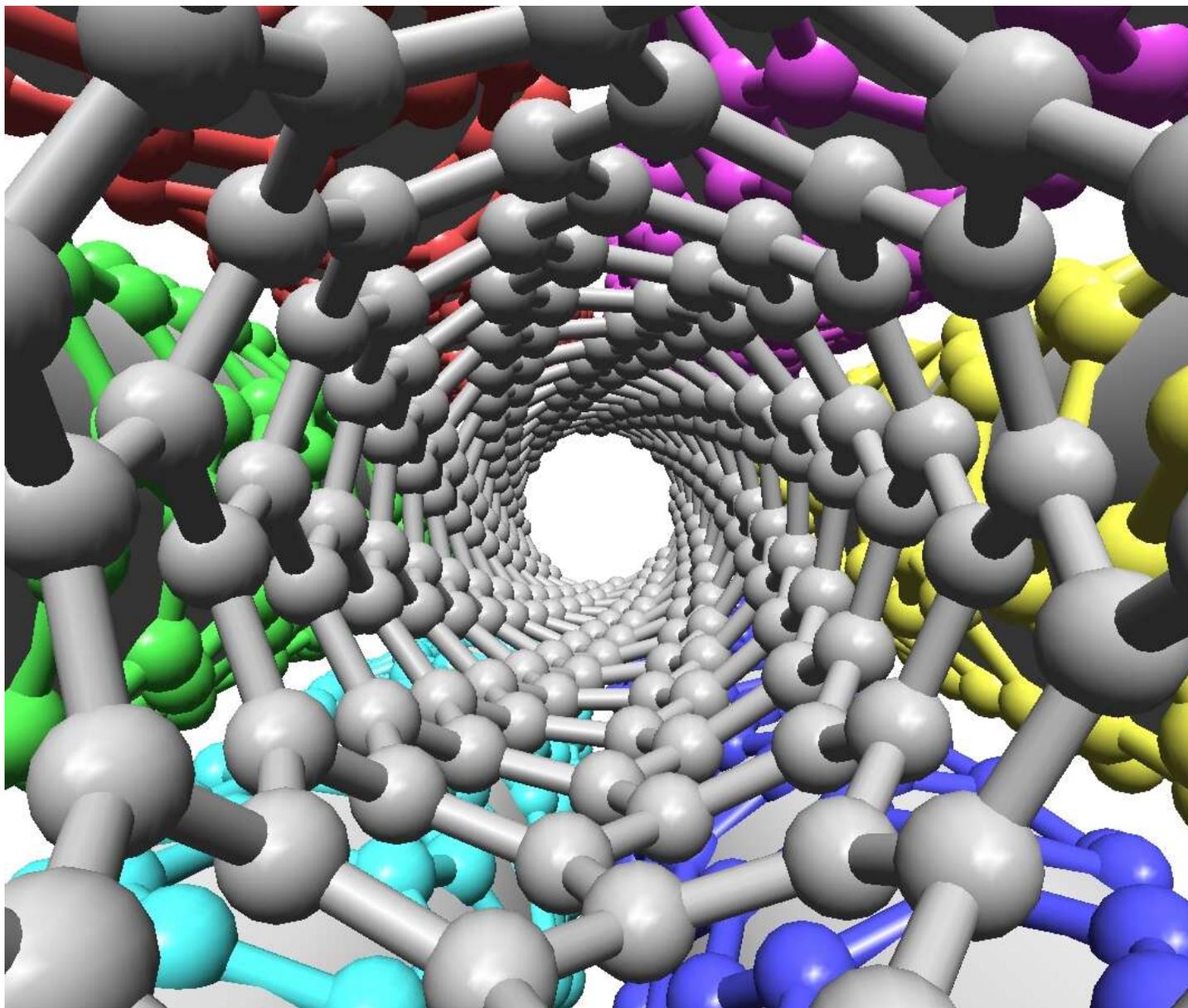


A bundle of seven  $\{7,3\}$  nanotubes

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# *Inside {5,3} Nanotube*

---

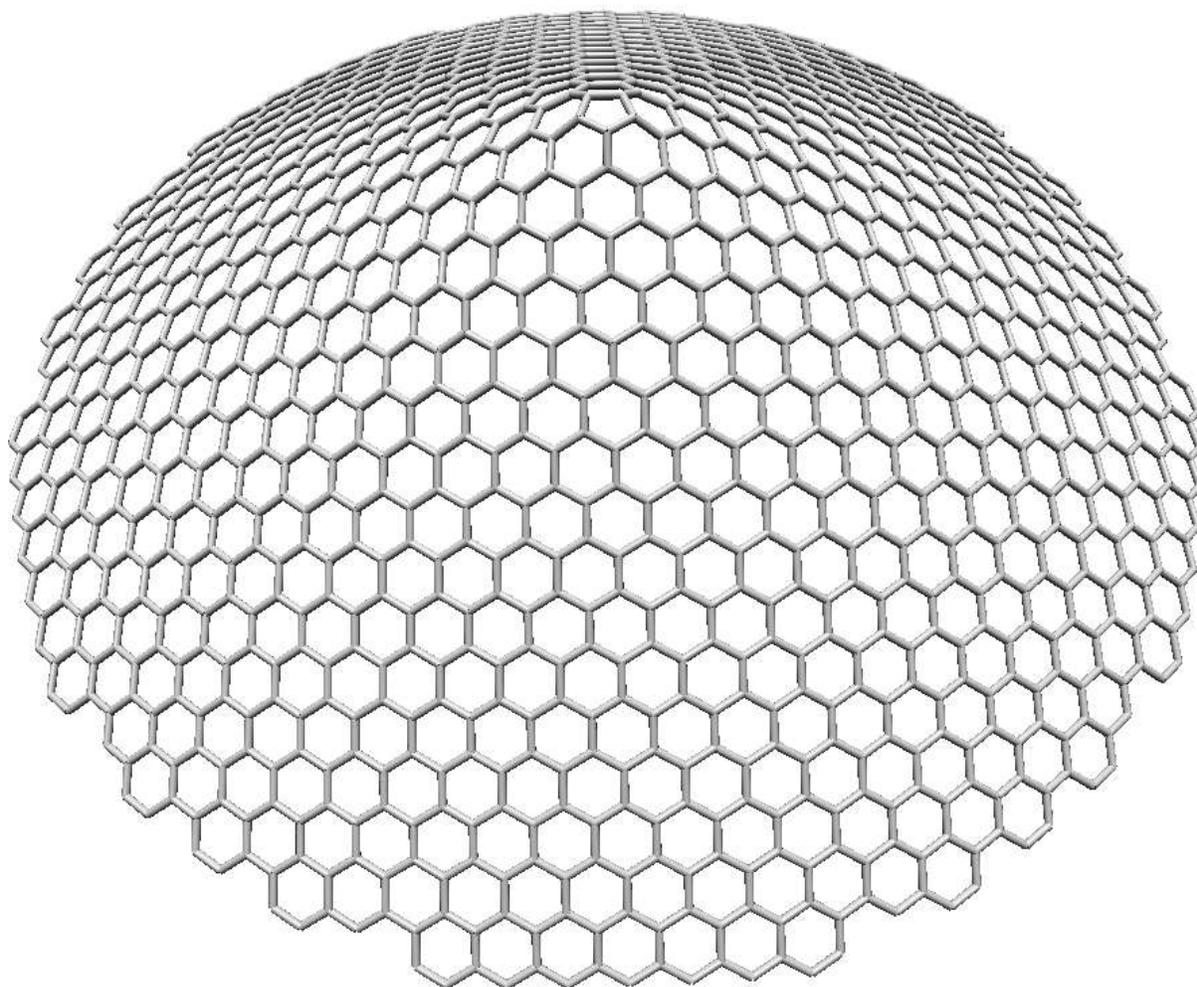


Looking inside a bundle of {5,3} nanotubes

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# *60° - Nanocone*

---

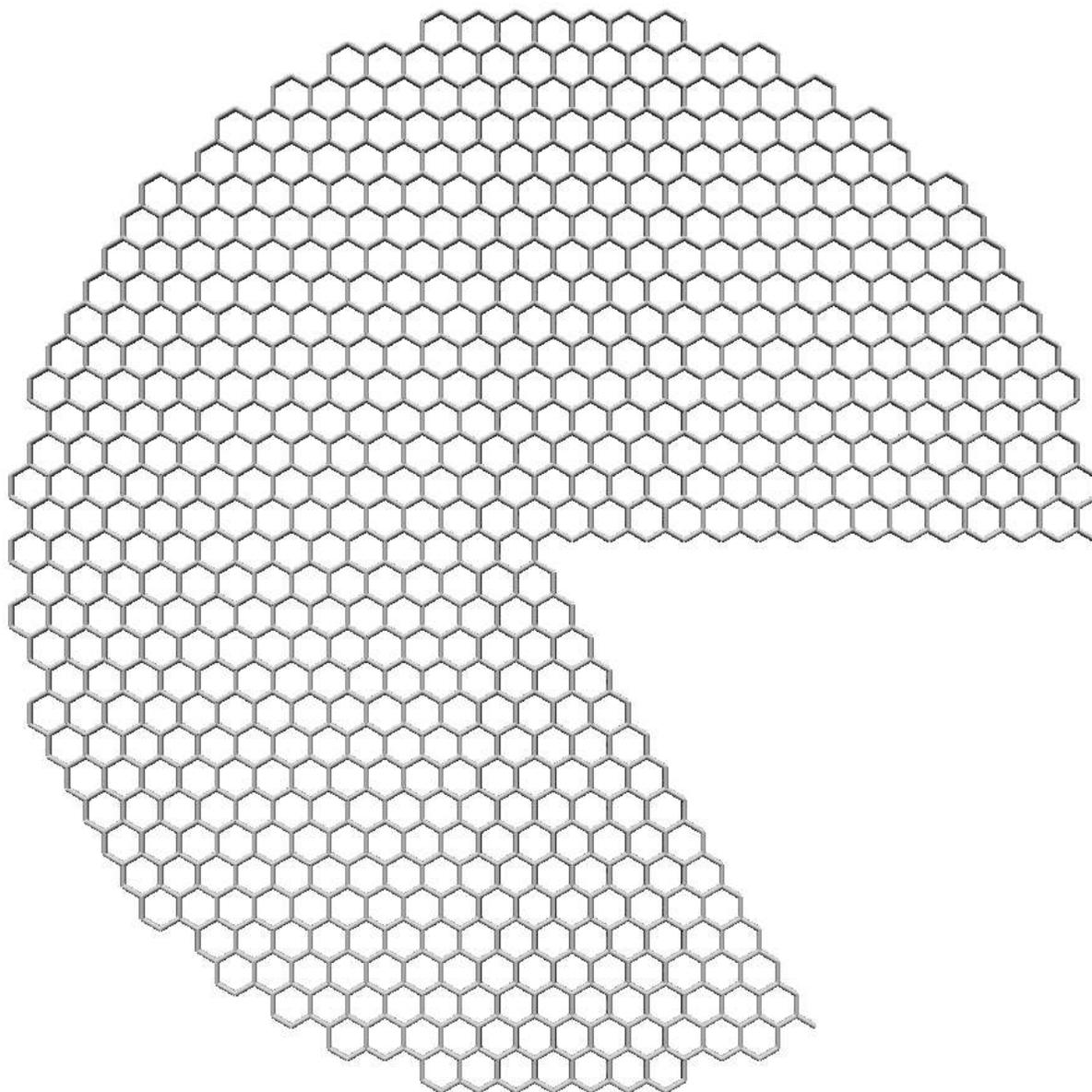


Disclination angle  $60^\circ$   
Cone height 20 Å

---

# *60° - Nanocone Sheet*

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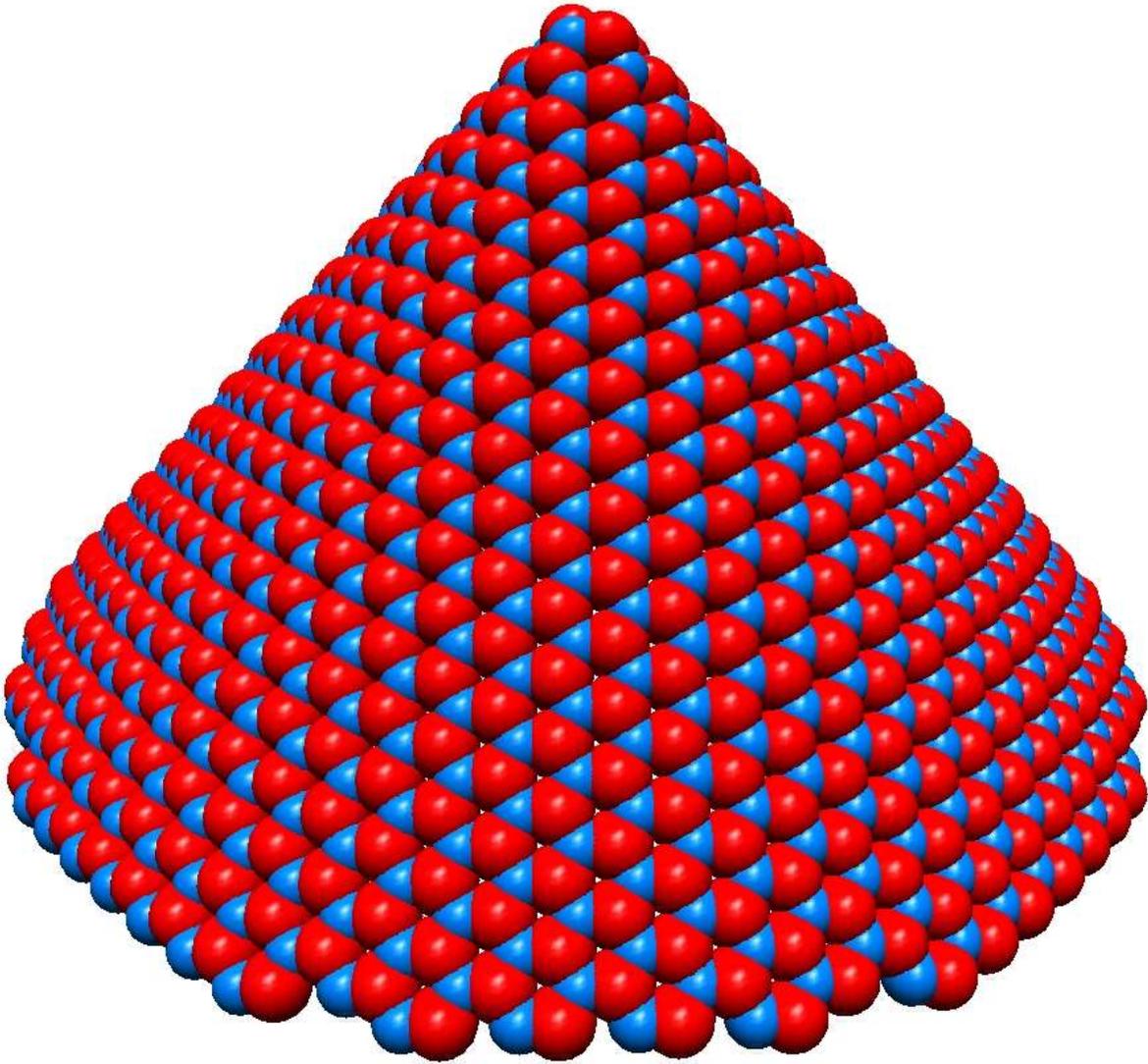


Disclination angle  $60^\circ$   
Creates a cone of height  $20 \text{ \AA}$

---

# *120° - Nanocone*

---

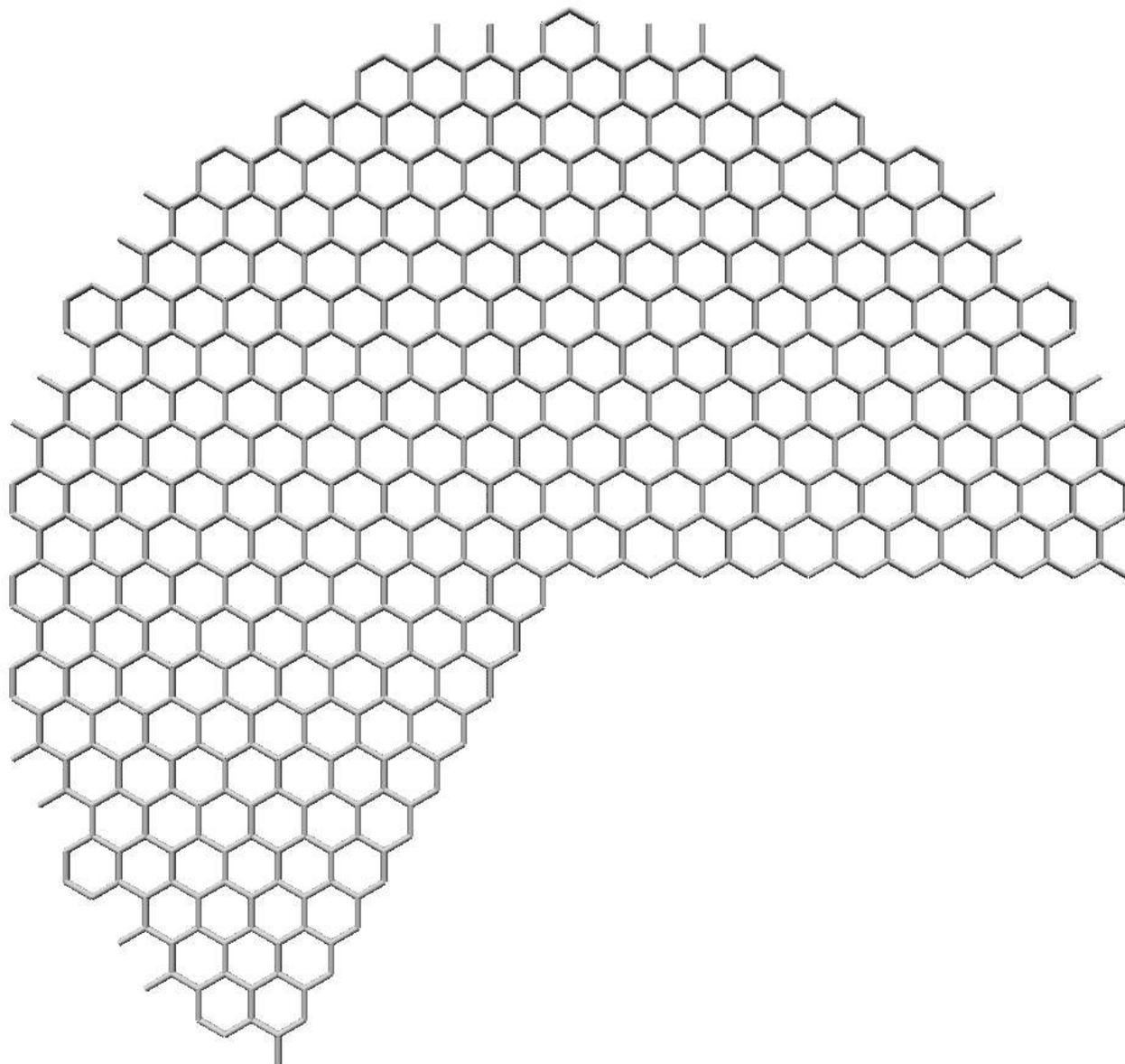


Disclination angle  $120^\circ$   
Cone height  $30 \text{ \AA}$

---

# *120° - Nanocone Sheet*

---

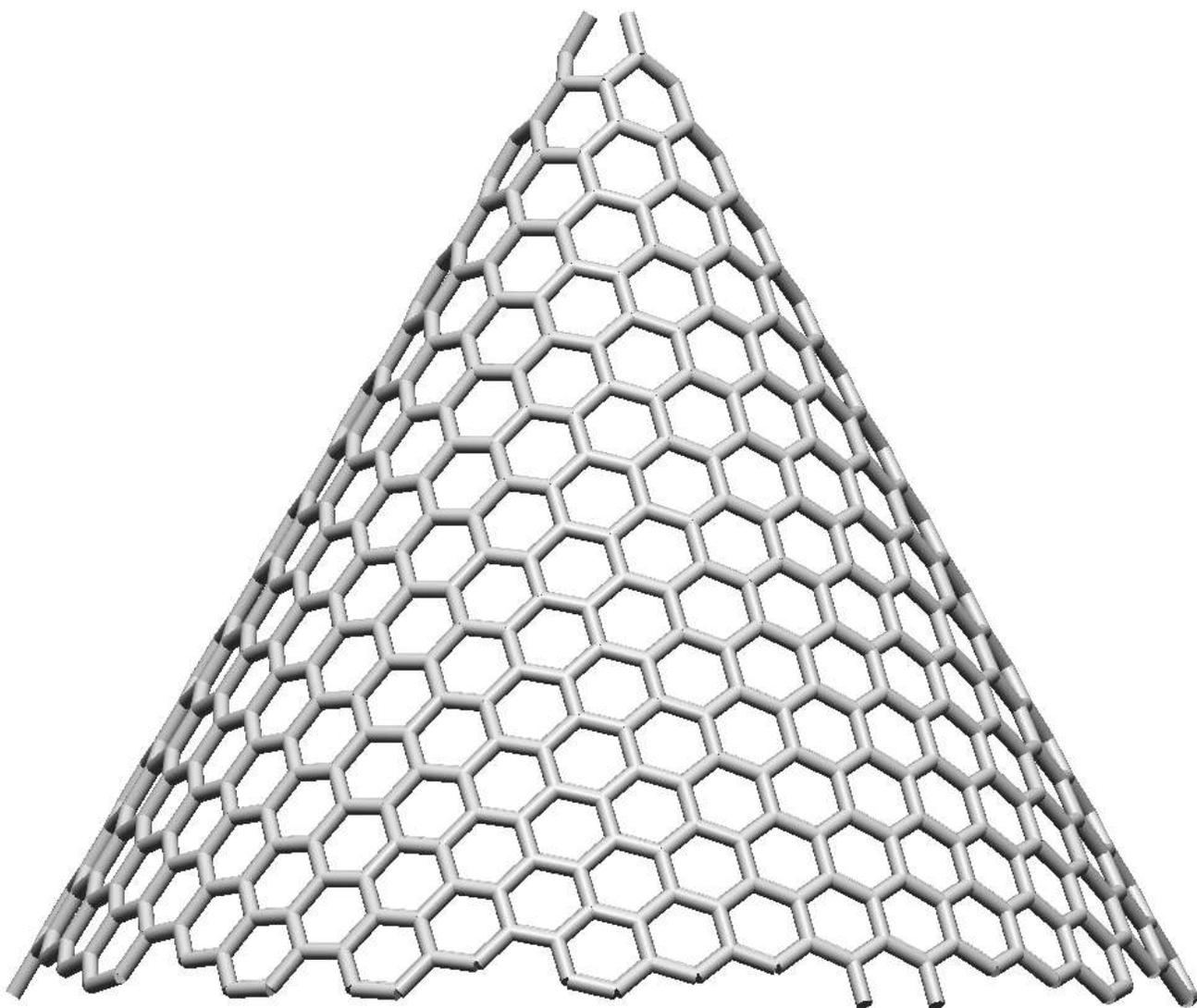


Disclination angle  $120^\circ$   
Creates a cone of height  $20 \text{ \AA}$

---

# *180° - Nanocone*

---

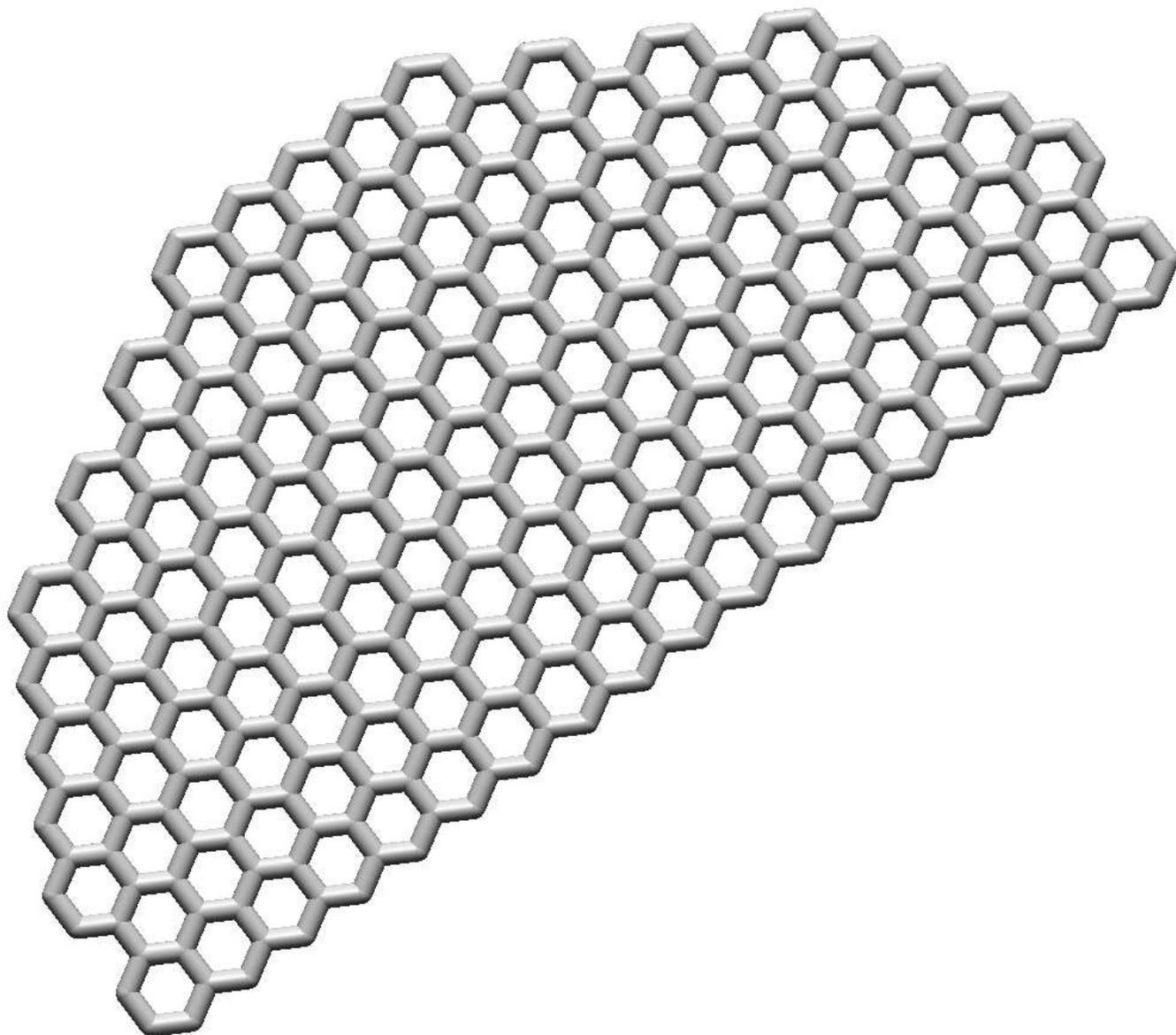


Disclination angle  $180^\circ$   
Cone height 30 Å

---

# *180° - Nanocone Sheet*

---

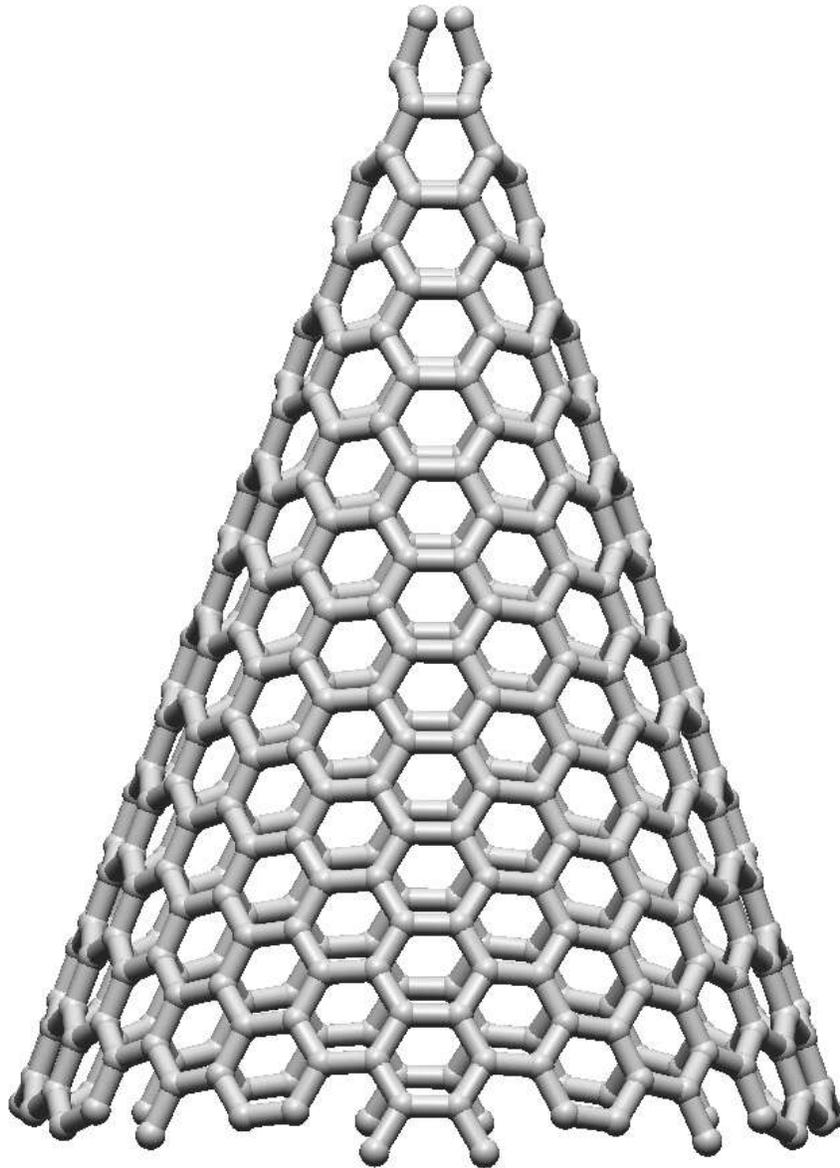


Disclination angle  $180^\circ$   
Creates a cone of height  $20 \text{ \AA}$

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# *240° - Nanocone*

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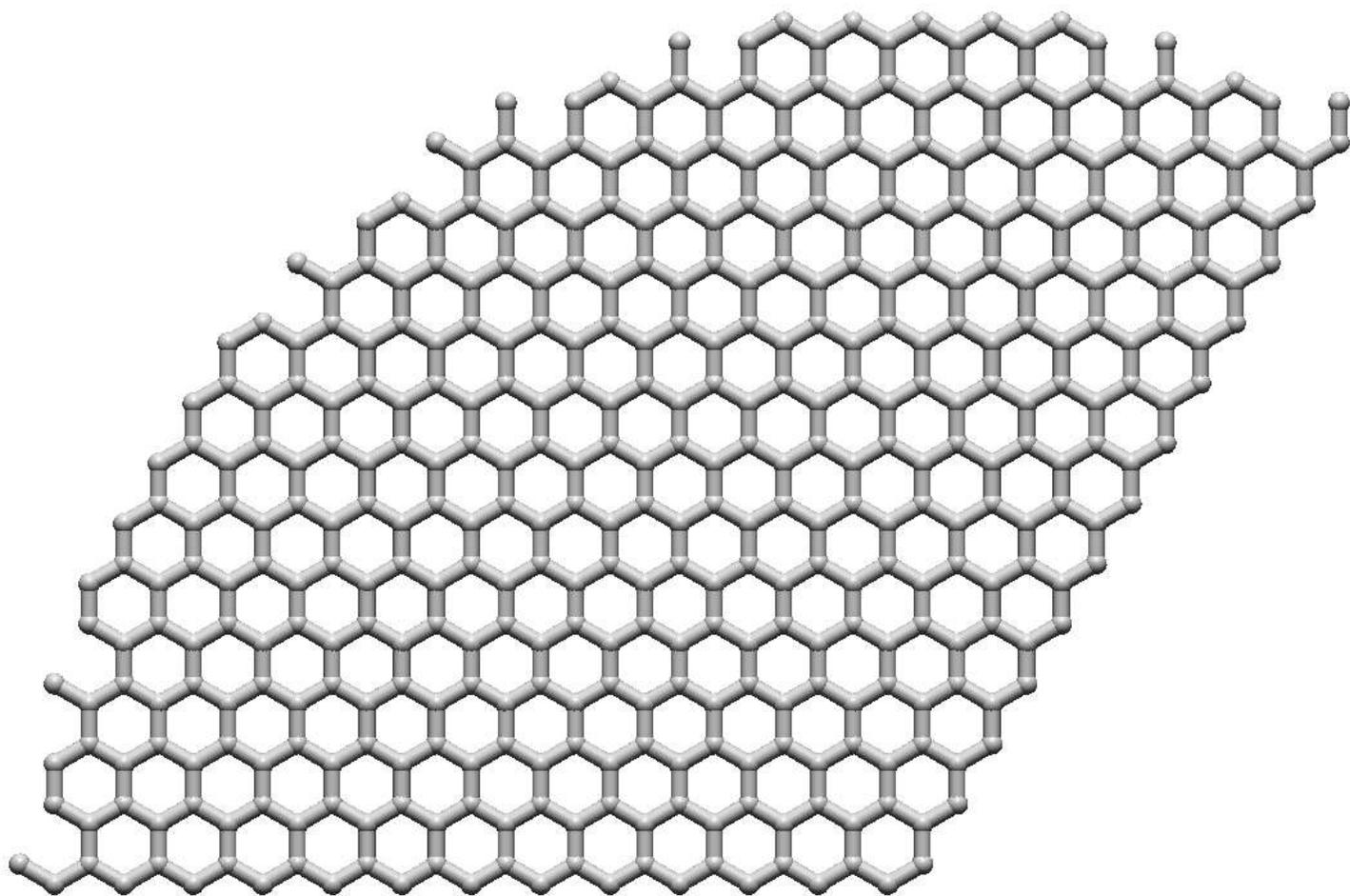


Disclination angle  $240^\circ$   
Cone height 30 Å

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# *240° - Nanocone Sheet*

---

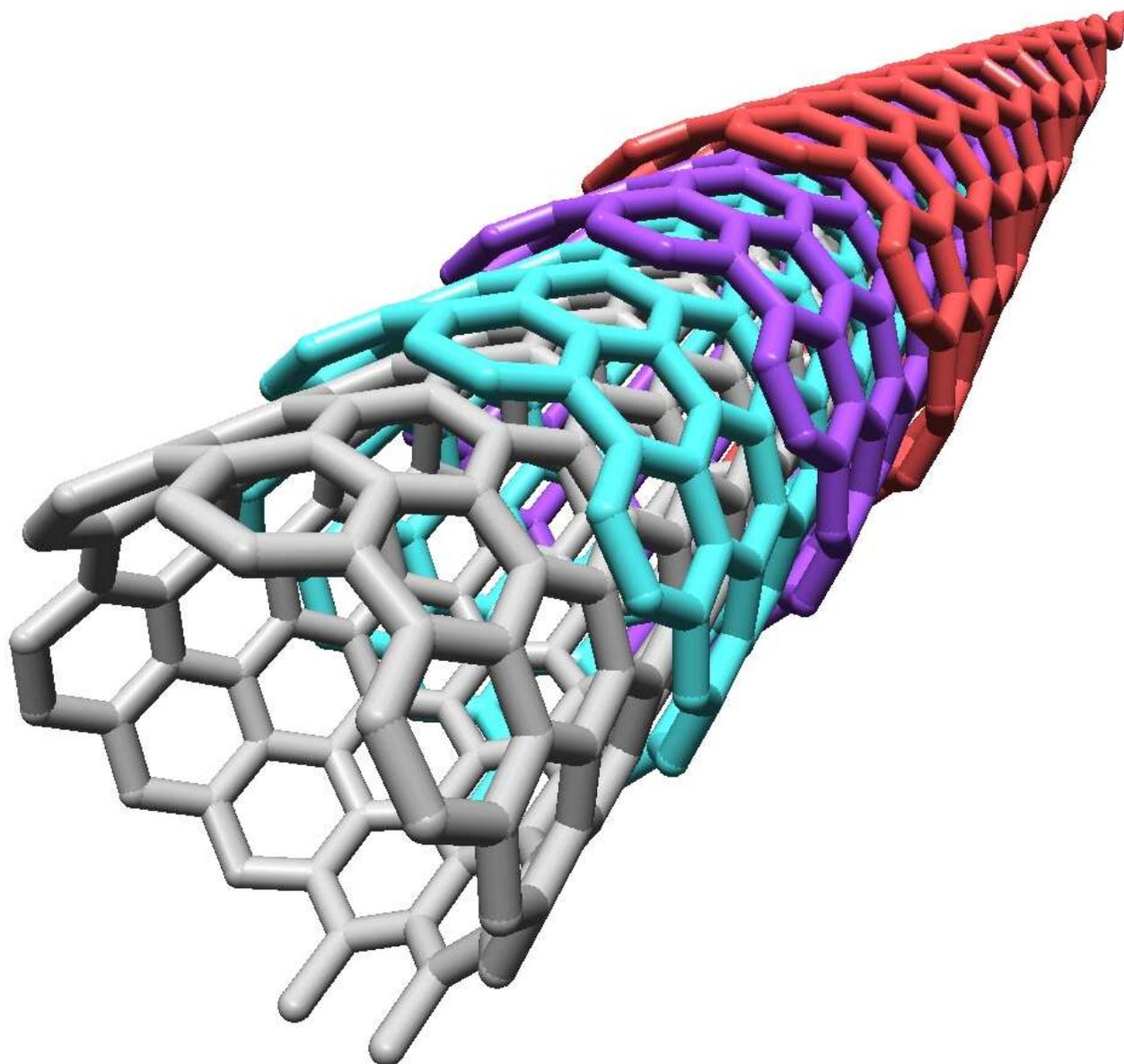


Disclination angle  $240^\circ$   
Creates a cone of height  $30 \text{ \AA}$

---

# *300° - Nanocone Stack*

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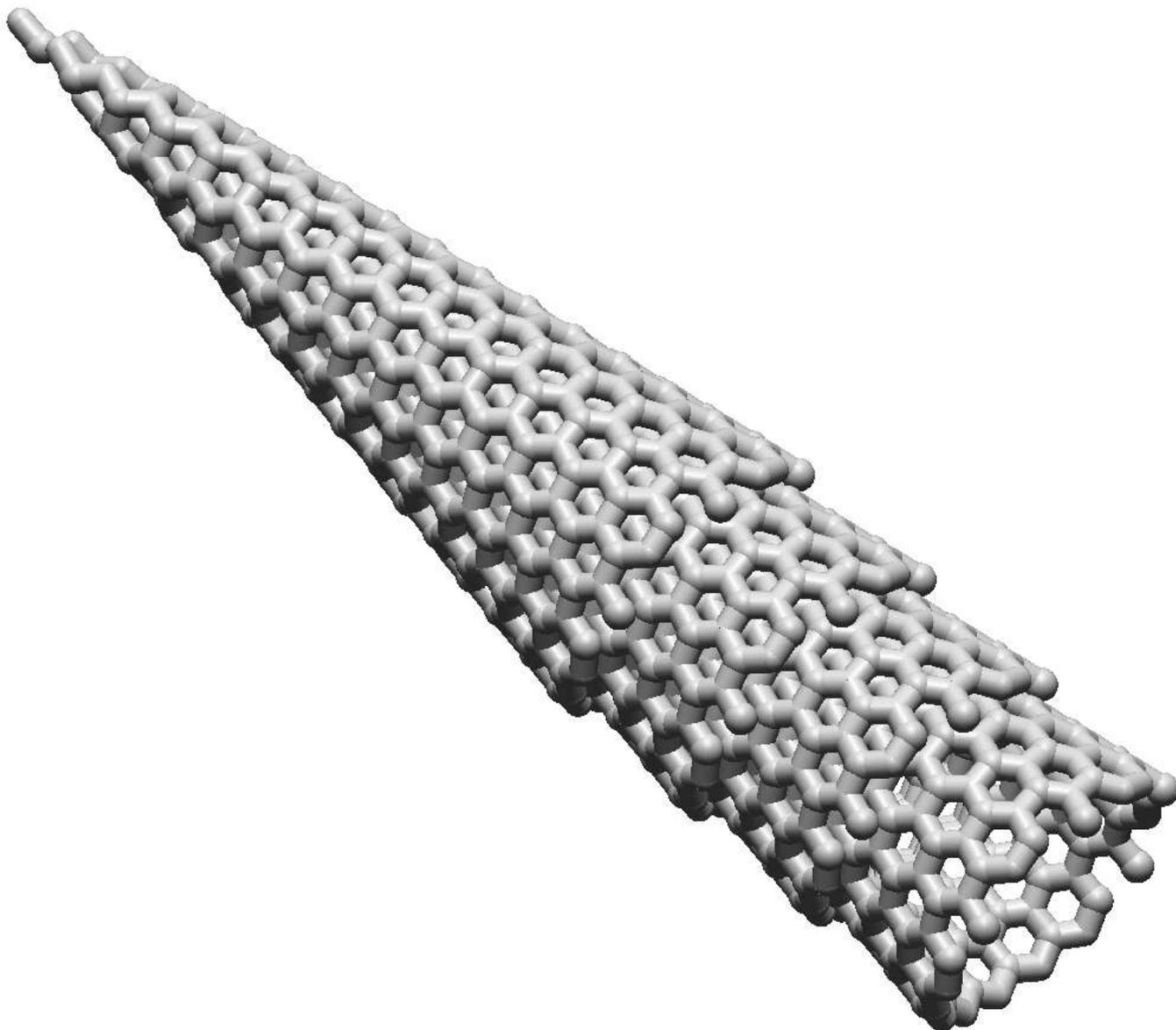


Disclination angle  $300^\circ$   
Four cones of height  $30 \text{ \AA}$

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# *300° - Nanocone Stack*

---

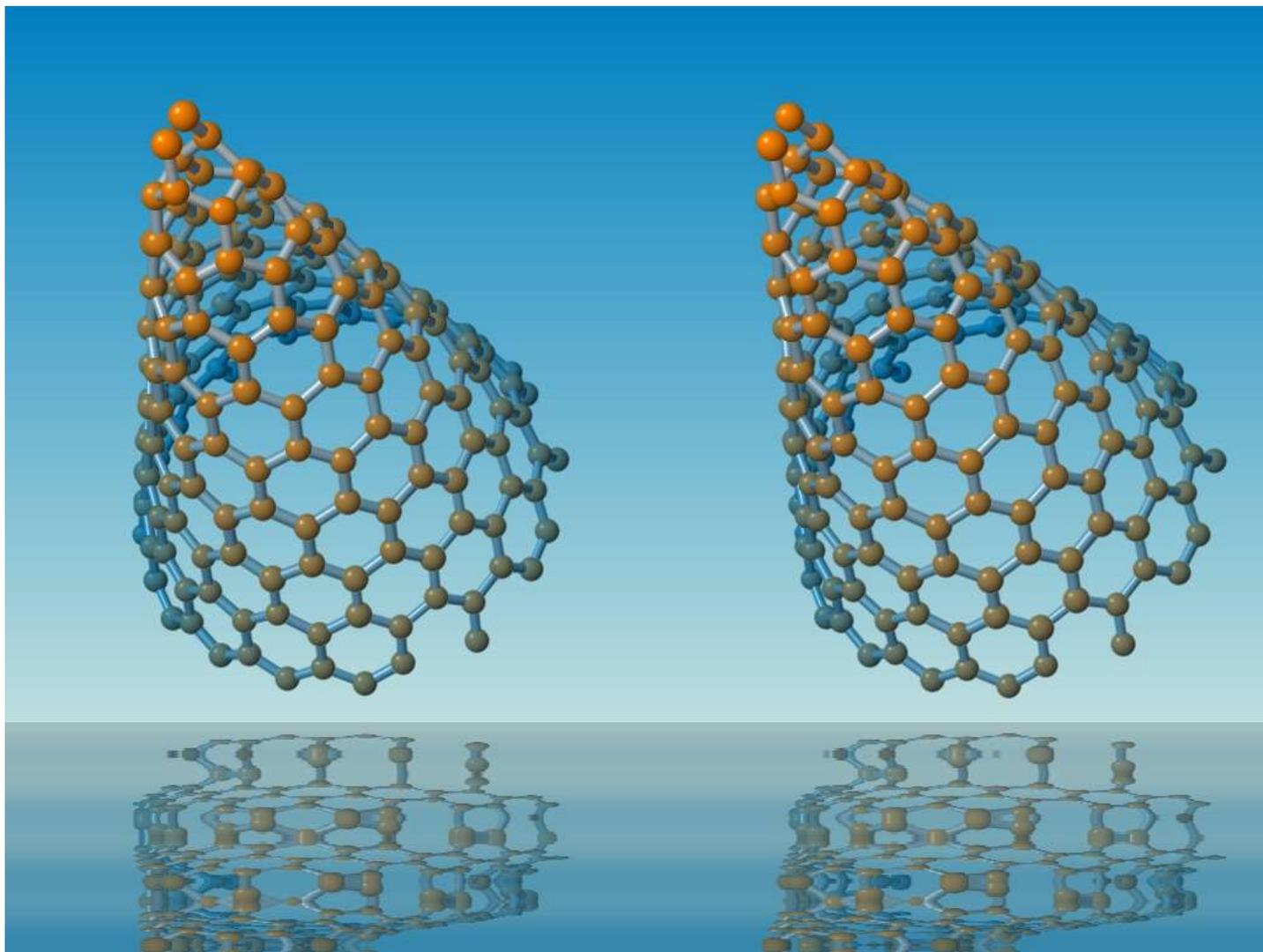


Disclination angle 300°  
Four cones of height 40 Å

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# *Nanocone Stereo Pair*

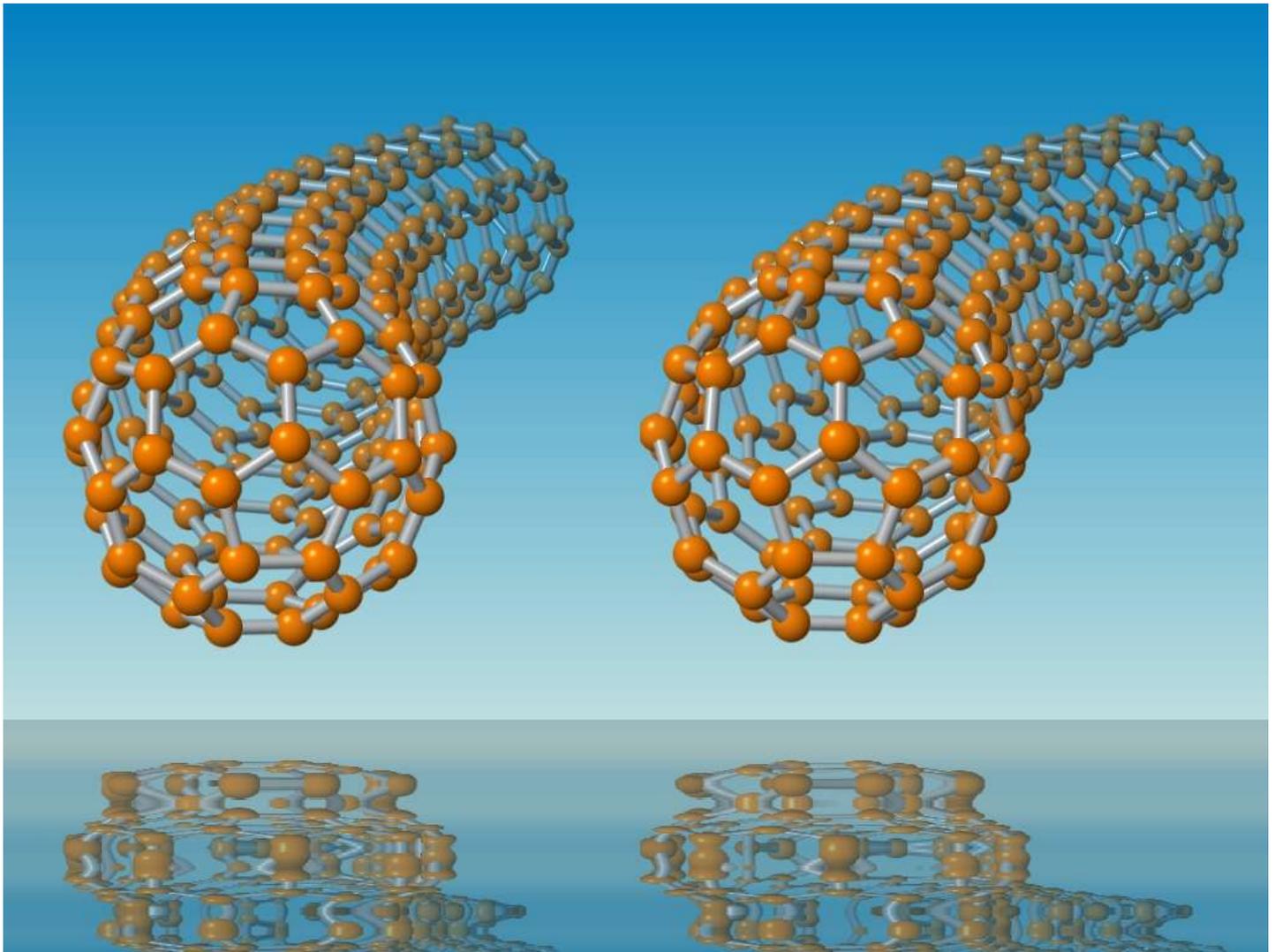
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Disclination angle  $240^\circ$ , Cone height 20 Å, Stereo view (relaxed-eye view)  
This image was created with JPOWD from MDI ([www.materialsdata.com](http://www.materialsdata.com))

# *Nanotube Stereo Pair*

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

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# *Disclaimer*

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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](http://jcrystal.com/steffenweber/gallery/NanoTubes/NanoTubes.html)  
[jcrystal.com/steffenweber/gallery/NanoTubes/NanoCones.html](http://jcrystal.com/steffenweber/gallery/NanoTubes/NanoCones.html)

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