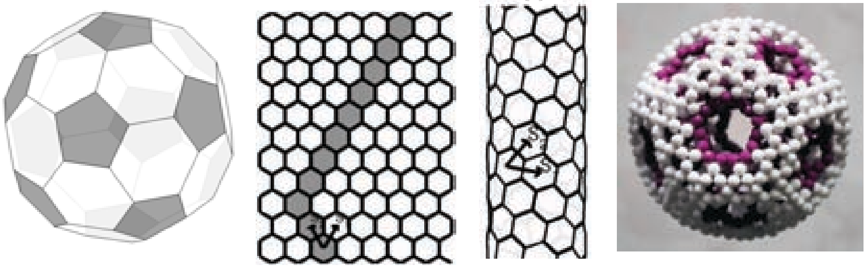
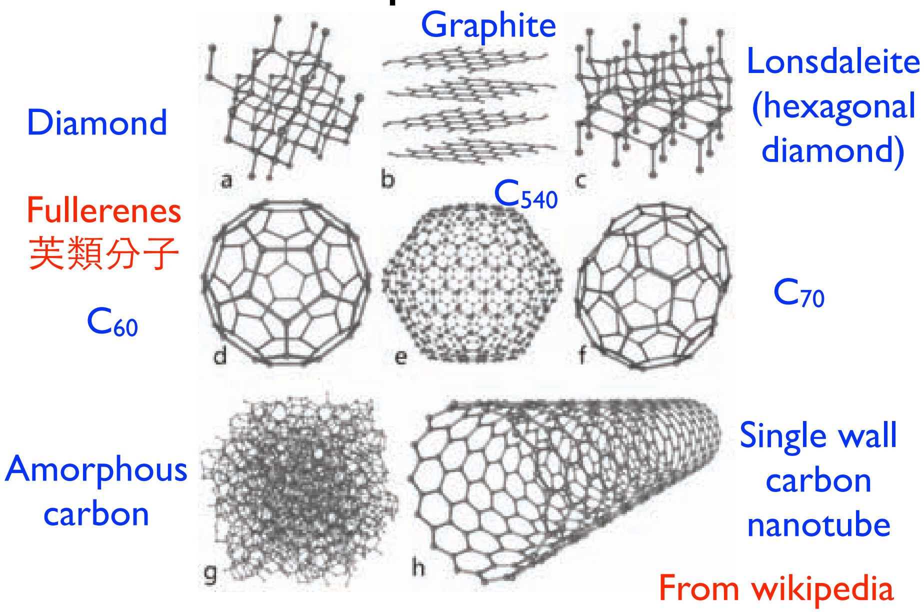
Fullerenes, carbon nanotubes, and other exotic graphitic materials: structures and models

Bih-Yaw Jin 金必耀
Department of Chemistry, National Taiwan University

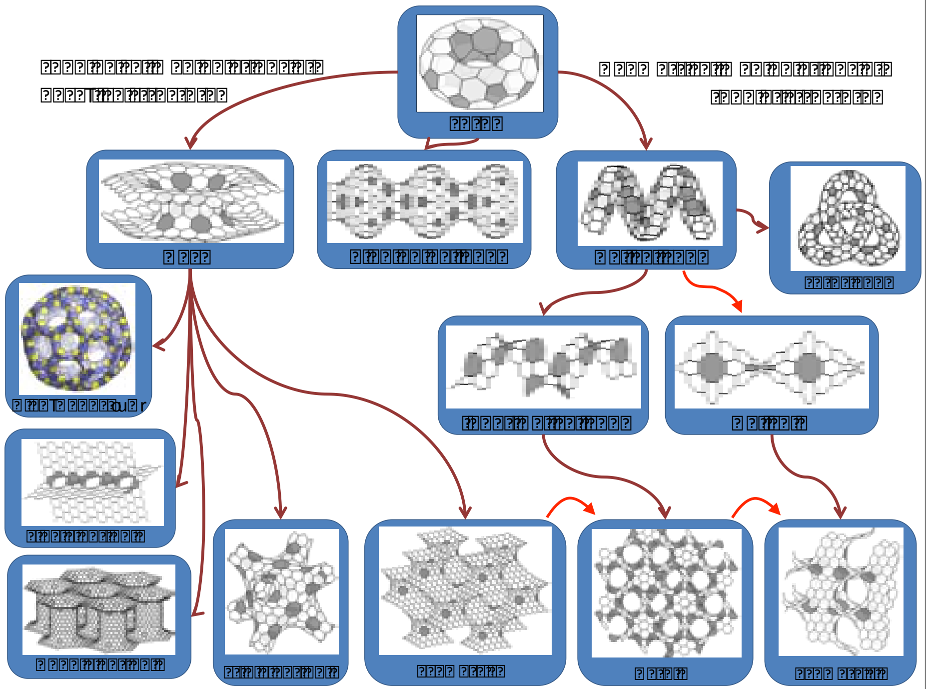


清華大學物理系 May 2, 2011

Allotropes of carbon

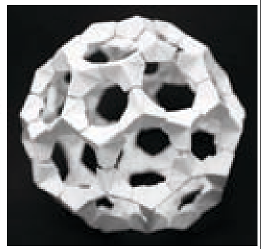


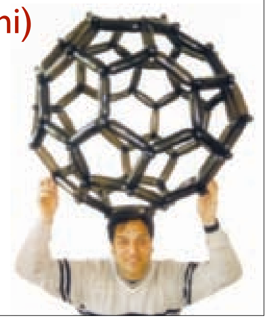
From wikipedia



Physical models

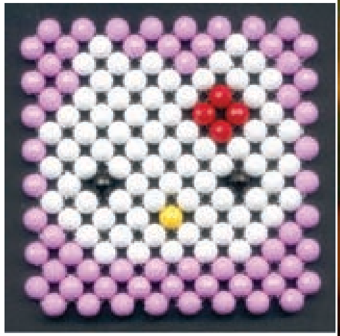
- Ball-and-Stick model
- Space-Filling model
- Wire model
- Paper-folding model (Modular Origami)
- Paper-cutting model
- Balloon model
- Rapid prototyping





Traditional Beading

1D

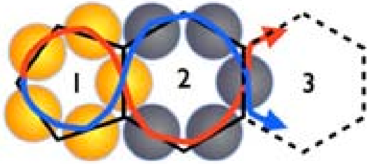


2D

3D

Stereobeading: Animal

Figure-Eight Stitch (八字編)

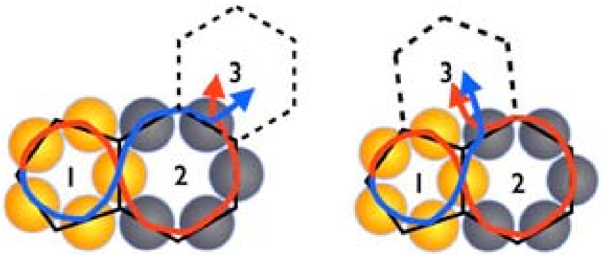


Japan

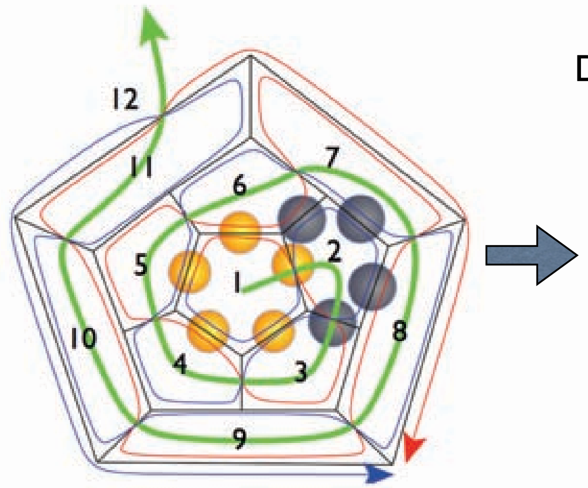
Hachinoji-Ami Stitch

West

Right-Angle Weave



Schlegel's diagram and beading pattern



Dodecahedron (C_{20})

tangent spheres

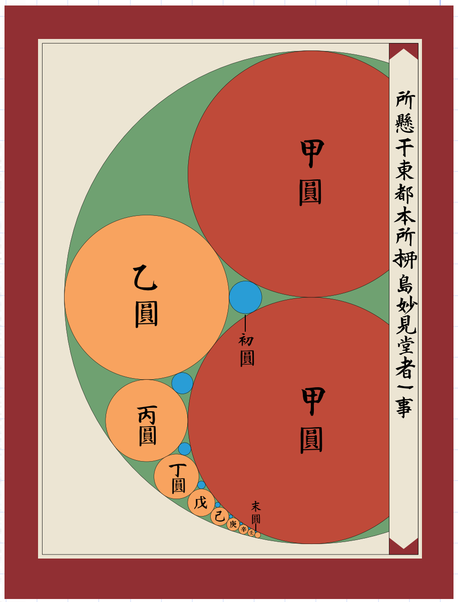
□□□□□□□□□□□□

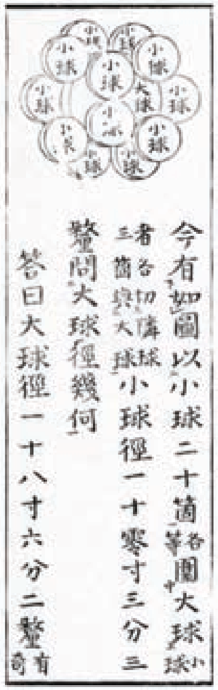
Scientific American 2005

Japanese Temple Geometry

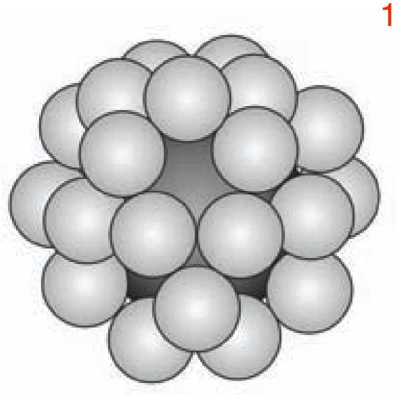
During Japan's period of national seclusion (1639–1854), native mathematicians thrived, as evidenced in sangaku—wooden tablets engraved with geometry problems hung under the roofs of shrines and temples

By Tony Rothman, with the cooperation of Hidetoshi Fukagawa





1796



三十個の球の外接問題

算法助術（天保十二年）

Let a large sphere be surrounded by 30 small, identical spheres, each of which touches its four small-sphere neighbors as well as the large sphere. How is the radius of the large sphere related to that of the small spheres?

Stereobeading for molecules

Jin, B.-Y.*; Chuang, C.; Tsoo, C.-C. Construction of Physical Models for Arbitrary Fullerenes with Beads: Realization of Tangent-Sphere Model *J. Chin. Chem. Soc.* **2010**, 57, 316-324.

【化學奇境】一線千珠走入分子世界

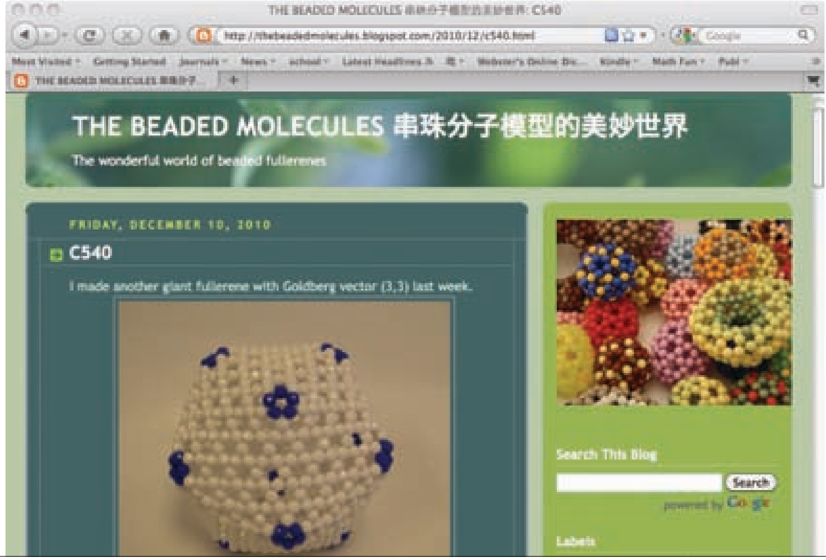
漫遊分子奇境·第五講 特稿

"CASE □ Center for the Advancement of Science Education

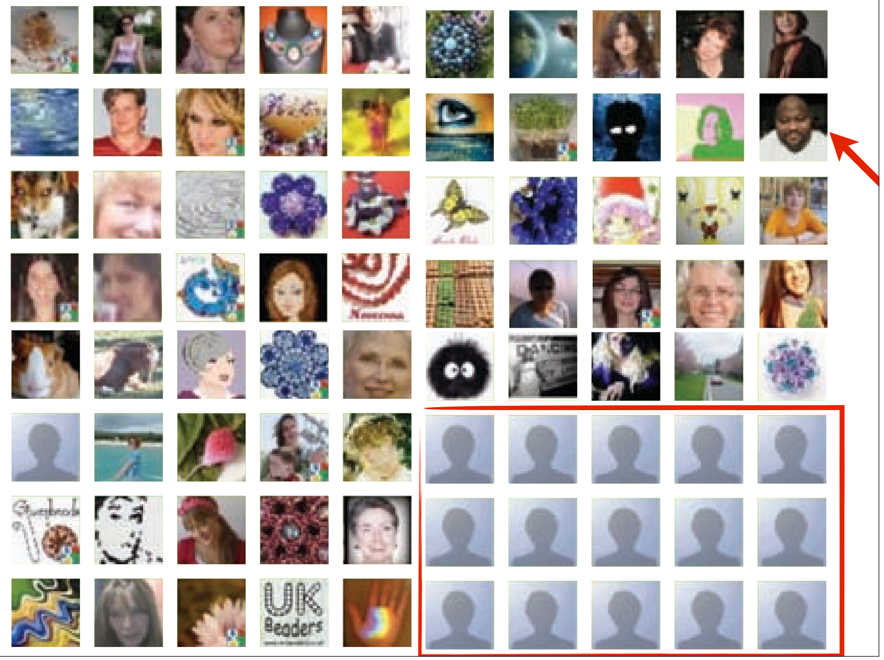
□□ □ □□□□□□□□□□□□□□"

The beaded molecules blog

http://thebeadedmolecules.blogspot.com/

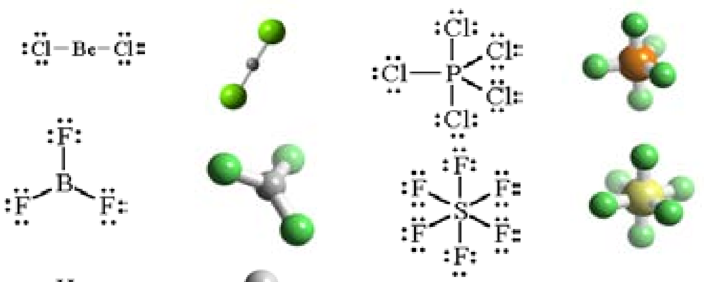


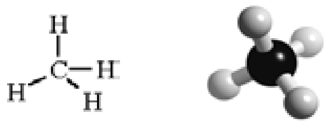
Followers of my blog (84)



Geometry of molecules

Valence Shell Electron Pair Repulsion (VSEPR) model:
Local structure of a molecule is determined by VSEPR.



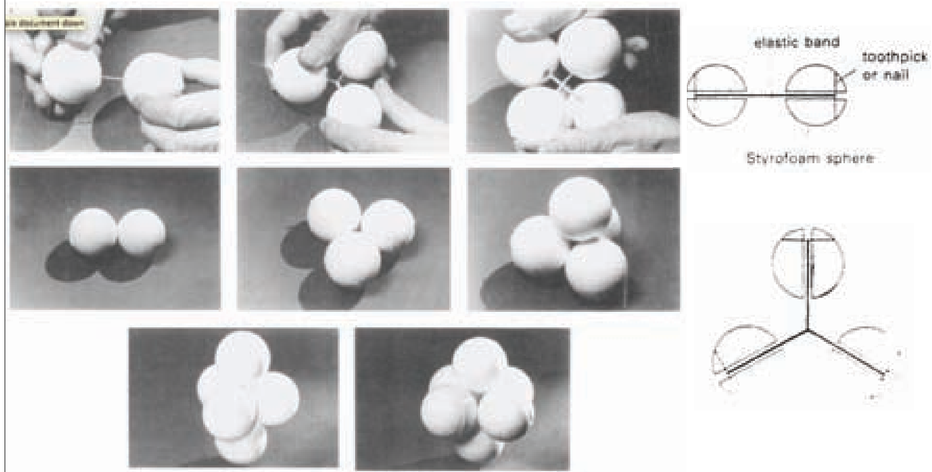


Ronald J. Gillespie (1957)

Bead model is possibly one of vey few physical models that really mimic microscopic force fields.

Styrofoam sphere model

The Electron-pair Domain Model (tangent sphere model)



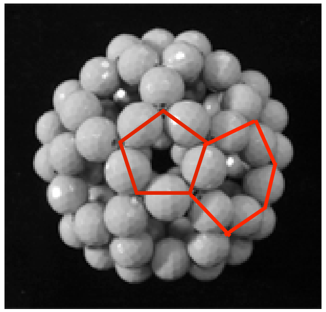
Ronald J. Gillespie, The VSEPR Model Revisited . Chem. Soc. Rev. 1992, 60.

Balloon model

http://balloonmolecules.com/

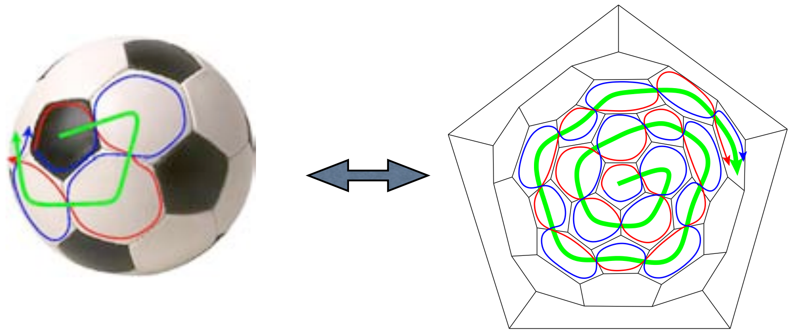
Vi Hart, Proceeding of Bridges 2010

Beaded Buckyball



- Bead Representation = Bond Representation
- 90 beads are needed for C_{60} $$60 \times 3/2 = 90$$
- Beaded fullerene represents the bond network

Weaving code = Spiral Code



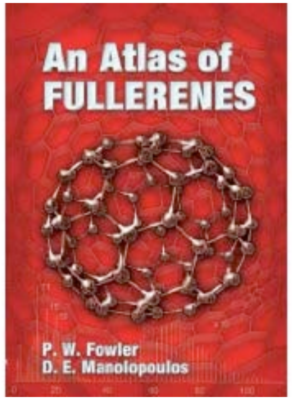
planar graph

- C_{60}: [1 7 9 11 13 15 18 20 22 24 26 32]
- For simple fullerenes without any hole, one can construct the corresponding bead model using spiral code only.

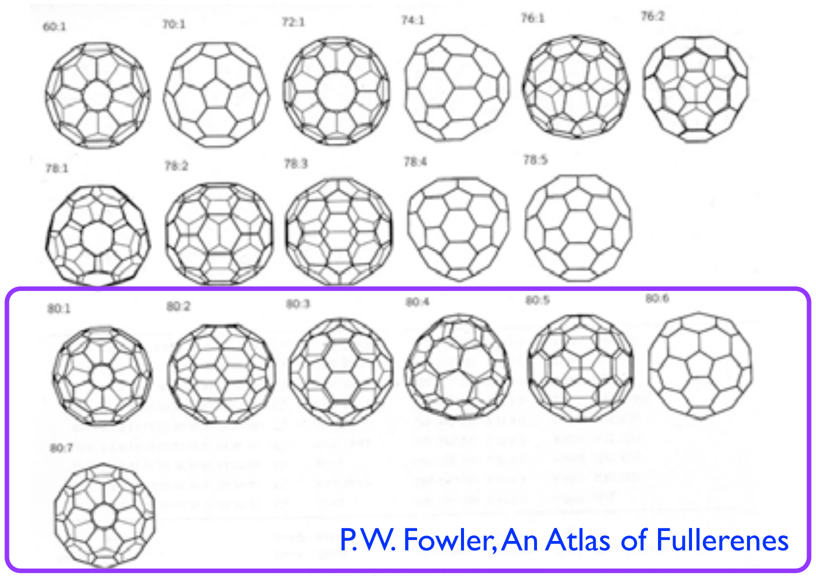
7 Isomers of C_{80}

Spiral Codes P.W. Fowler, An Atlas of Fullerenes

- [1 7 9 11 13 15 28 30 32 34 36 42]
- [1 7 9 11 13 18 25 30 32 34 36 42]
- [1 7 9 11 14 22 27 30 34 36 38 40]
- [1 7 9 11 14 23 28 30 33 35 37 39]
- [1 7 9 12 14 20 26 28 32 34 39 42]
- [1 7 10 12 14 19 26 28 32 34 39 42]
- [1 8 10 12 14 16 28 30 32 34 36 42]



Structures of Fullerenes



P.W. Fowler, An Atlas of Fullerenes

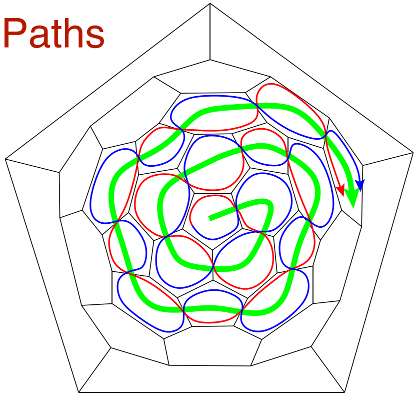
Point group: D_{5d}、D_2、C_{2v}、D_3、C_{2v}、D_{5h}、I_h

Minimal Length of String Required

- What is the minimal length of string for weaving a particular fullerene?
- Hamiltonian Circuits or Paths

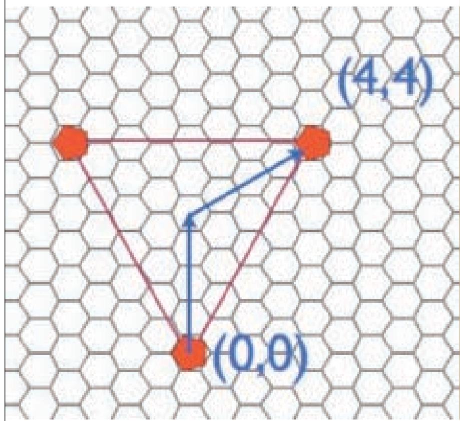
$$L_{min} = 2sNd + L_{ext}$$

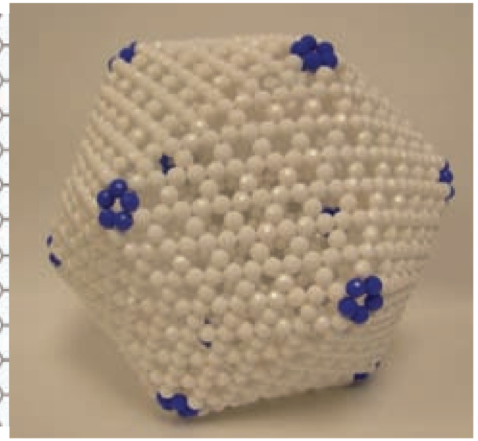
- d : diameter of bead.
- s = 1.1
- Lex: extra length



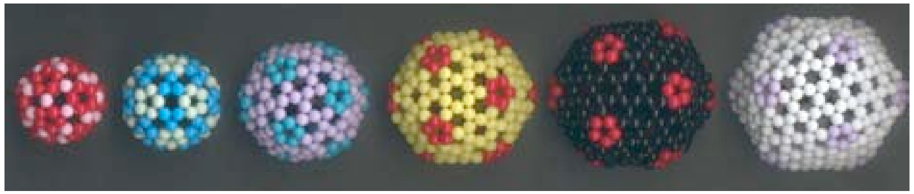
Goldberg Construction

Goldberg vector: (4, 4) ⇒ C_{960}



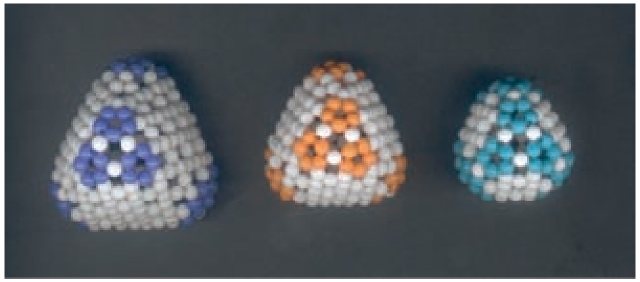


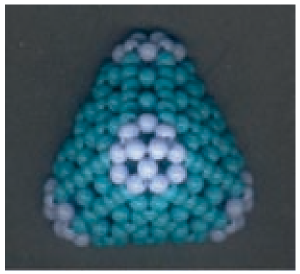
More icosahedral fullerenes



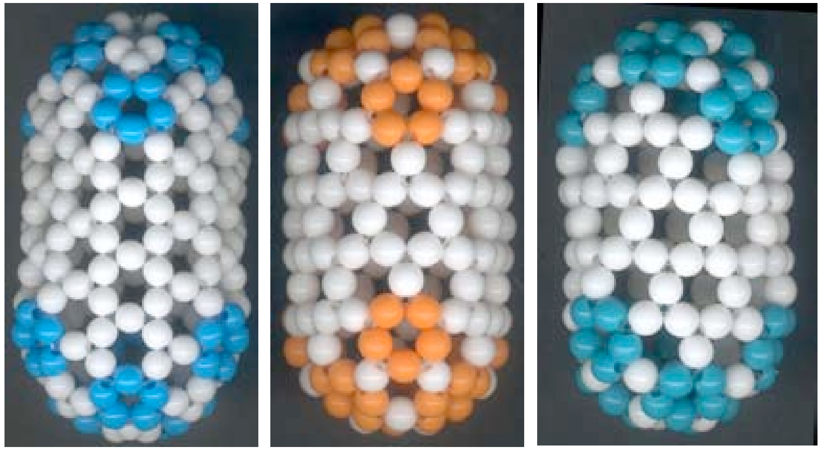
C_{60}	C_{80}	C_{140}	C_{180}	C_{240}	C_{260}
(1,1)	(2,0)	(2,1)	(3,0)	(2,2)	(3,1)

Truncated Tetrahedron





Endcappd carbon nanotubes



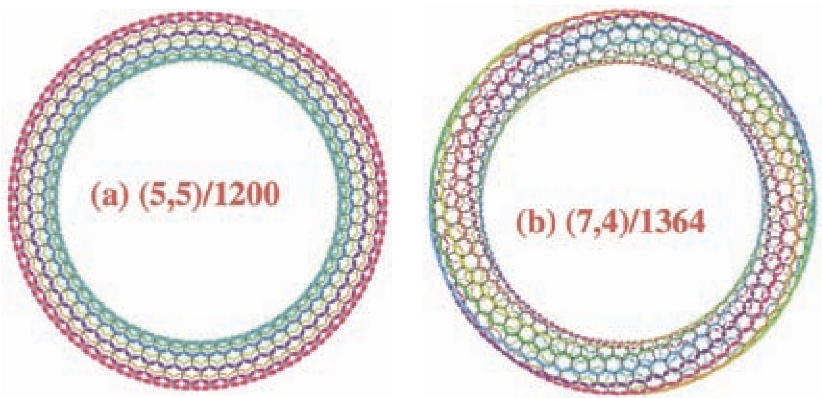
芙袋（Fullerene Bag）

VOLUME 88, NUMBER 21 PHYSICAL REVIEW LETTERS 27 MAY 2002

Colossal Paramagnetic Moments in Metallic Carbon Nanotori

Lei Liu,[1] G. Y. Guo,[2] C. S. Jayanthi,[1] and S. Y. Wu[1]
[1]Department of Physics, University of Louisville, Louisville, Kentucky 40292
[2]Department of Physics, National Taiwan University, Taipei, Taiwan 106

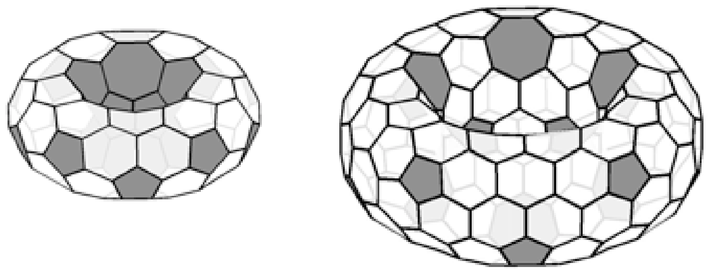
郭光宇教授



Small Toroidal Carbon Nanotubes (TCNTs)

Need nonhexagons to reduce strain energy!

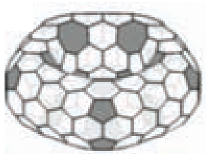
T120 T240



The genus of TCNTs

Euler-Poincare theorem, genus=g=1

$V-E+F=2-2g=0$

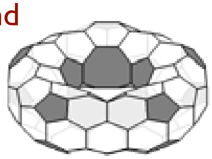


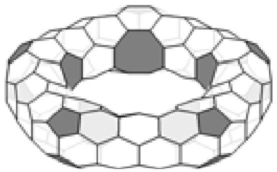
TCNTs with pentagons and heptagons

$N_5=N_7$

TCNTs with pentagons and octagons

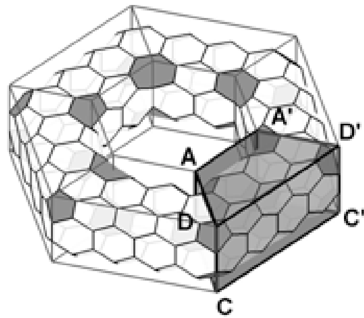
$N_5=2N_8$

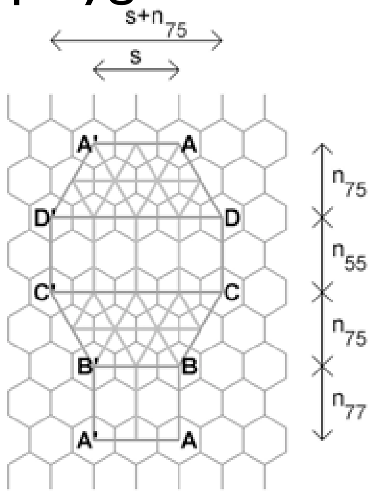




D_{nh}-TCNTs as polygonal Tori

$n_{\rm rot}=6$



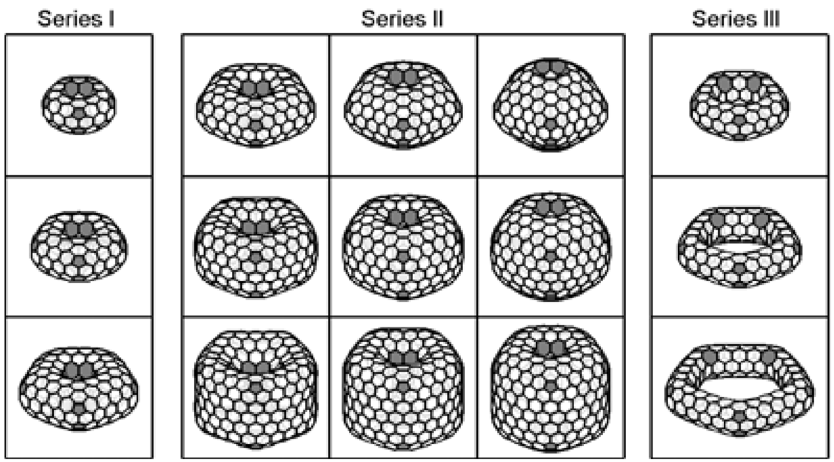


$(n_{75}, n_{77}, n_{55}, s)=(2, 1, 1, 2)$,
$(n_1,n_2)=(1, 0)$

We shall show that these tori are the patents of almost all high-symmetry TCNTs!

Tamura, R.; Ikuta, M.; Hirahara, T.; Tsukada, M. *Phys. Rev. B.* **2005**, *71*, 045418.

The shape space of D_{nh}-TCNTs



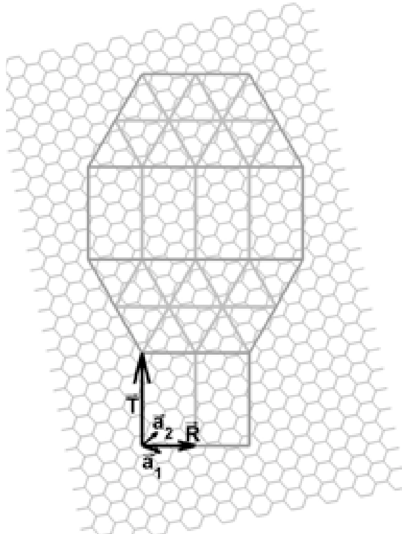
$n_{\rm rot}=5$

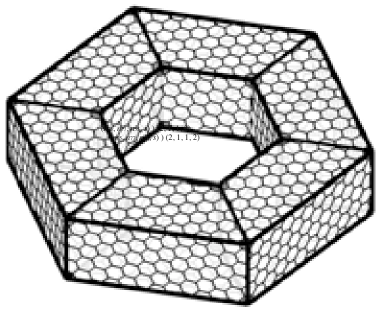
Chuang, C.; Fan, Y.-C.; Jin, B.-Y.* *J. Chem. Info. Model.* **2009**, 49, 361-368.

Change of Chiral Vector

Chirality shifting

$(n_{75}, n_{77}, n_{55}, s)=(2, 1, 1, 2)$,
$(n_1,n_2)=(2, 1)$



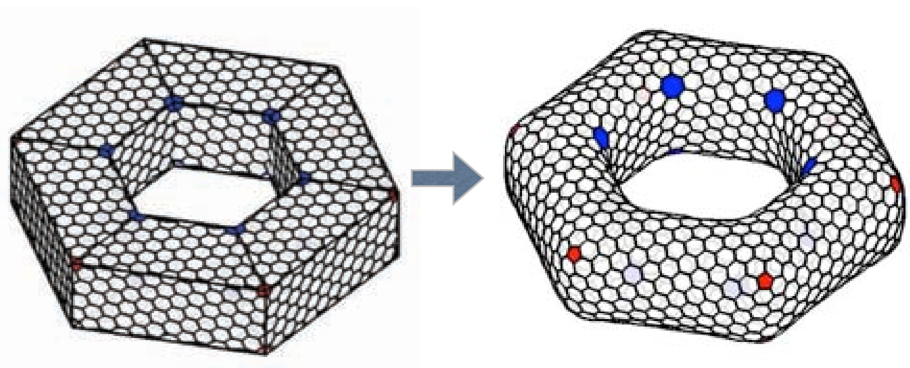


Goldberg inclusion

Chuang, C.; Fan, Y.-C.; Jin, B.-Y.* *J. Chem. Info. Model.* **2009**, 49, 361-368.

Optimized Chiral TCNT

$(n_{75}, n_{77}, n_{55}, s)=(2, 1, 1, 2)$,
$(n_1,n_2)=(2, 1)$



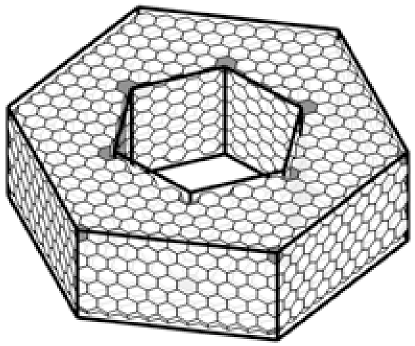
Chuang, C.; Fan, Y.-C.; Jin, B.-Y.* *J. Chem. Info. Model.* **2009**, 49, 361-368.

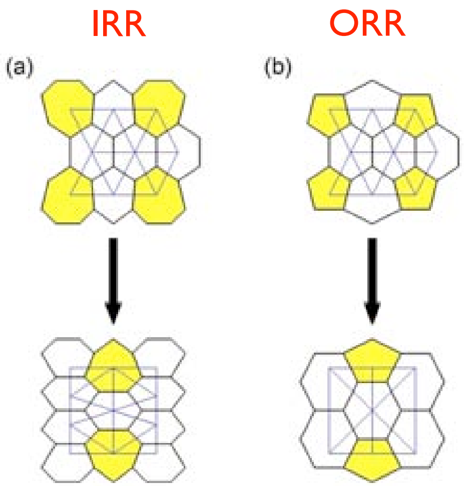
Three extra transformations

- Rim Rotation (RR)
  - Inner rim rotation (IRR)
  - Outer rim rotation (ORR)
- Horizontal Shift (HS)
  - Inner horizontal shift (IHS)
  - Outer horizontal shift (OHS)
- generalized Stone-Wales Transformation (gSWT)

Rim Rotation

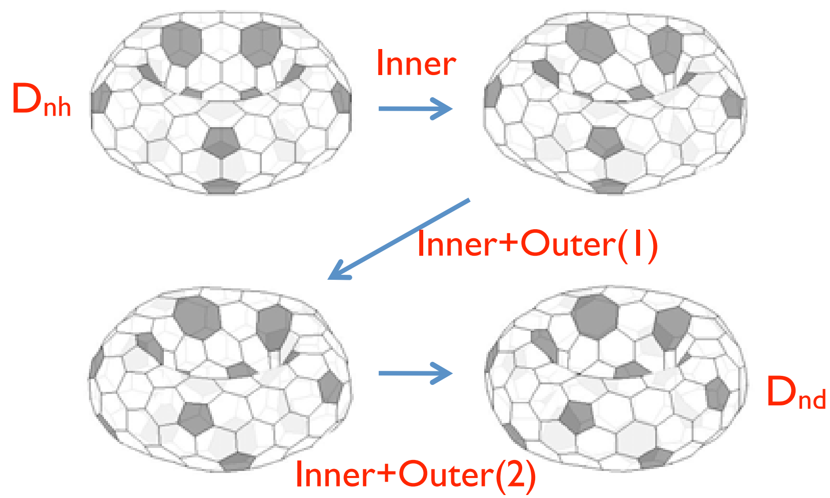
Inner rim rotation (IRR)





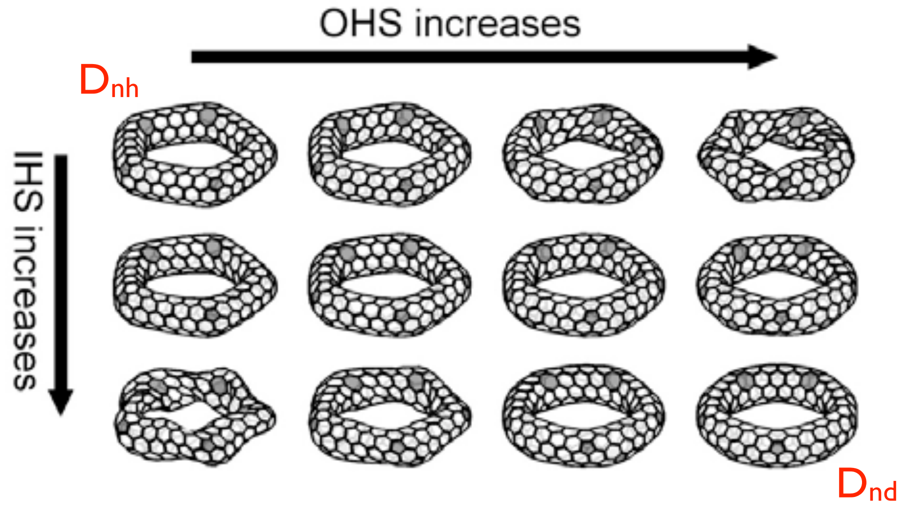
Chuang, C.; Fan, Y.-C.; Jin, B.-Y.* *J. Chem. Info. Model.* **2009**, 49, 361-368.

Horizontal Shift

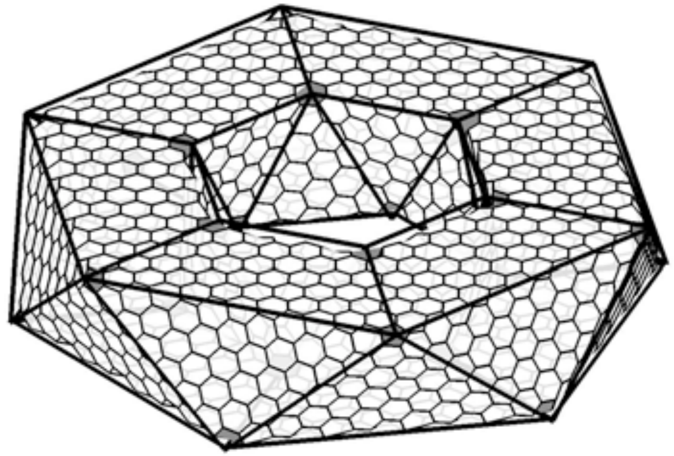


Isomerization between D_{nh} and D_{nd}

Horizontal Shift

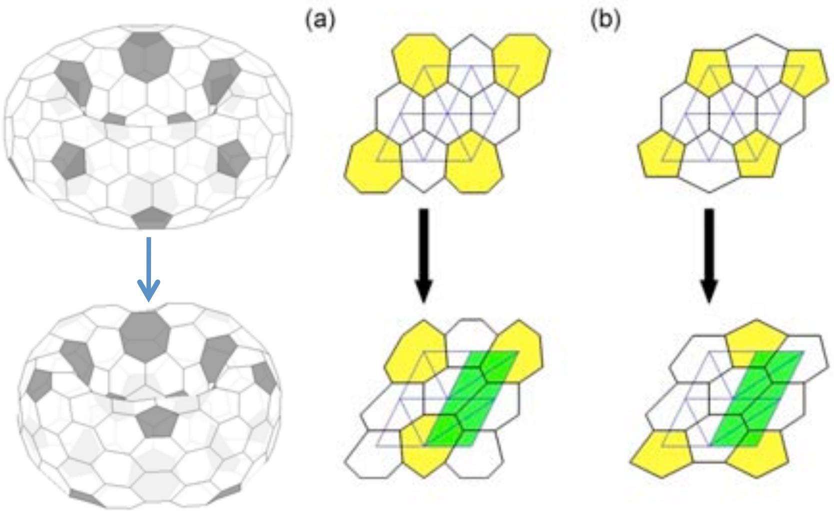


Antiprism: D_{nd} Isomers



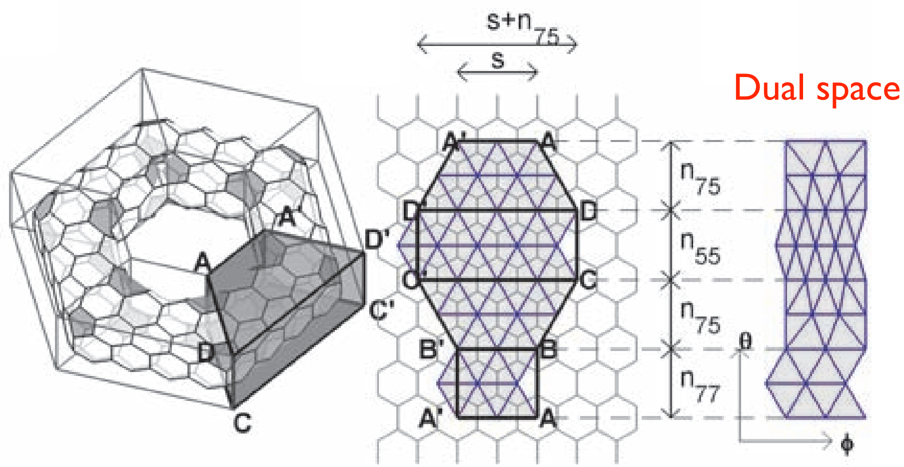
Chuang, C.; Fan, Y.-C.; Jin, B.-Y.* *J. Chem. Info. Model.* **2009**, 49, 361-368.

Isomerization: Generalized Stone-Wales Transformation



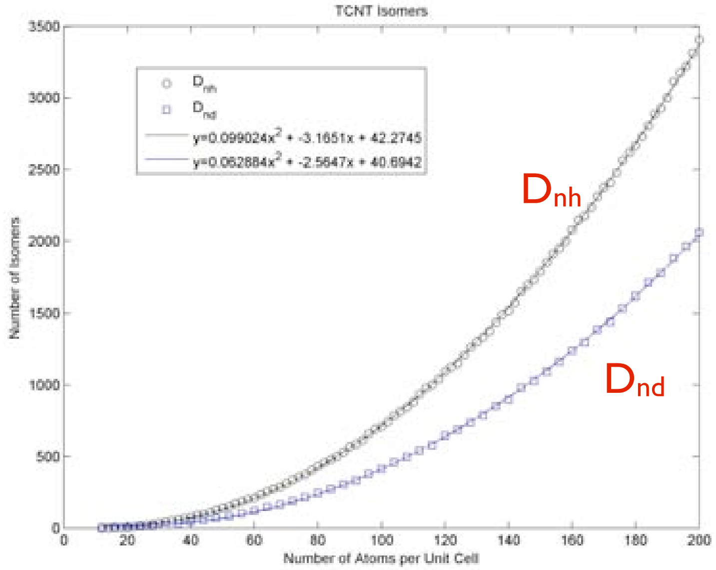
Avron, J.; Berger, J. Tiling rules for toroidal molecules. *Phys. Rev. A.* **1995**, *51*, 1146-1149.

Dual Space Representation



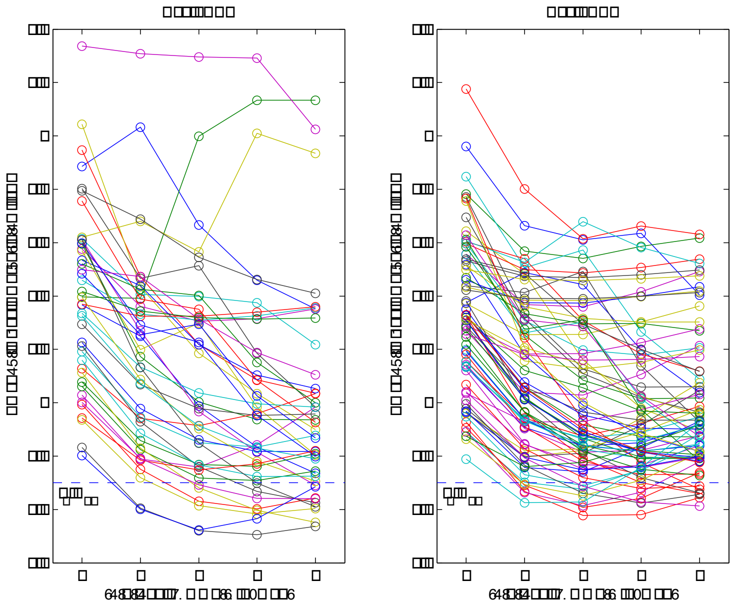
Chuang, C; Fan, Y.-C.; Jin, B.-Y.* *J. Chem. Info. Model.* **2009**, 49, 1679-1686.

Number of Isomers

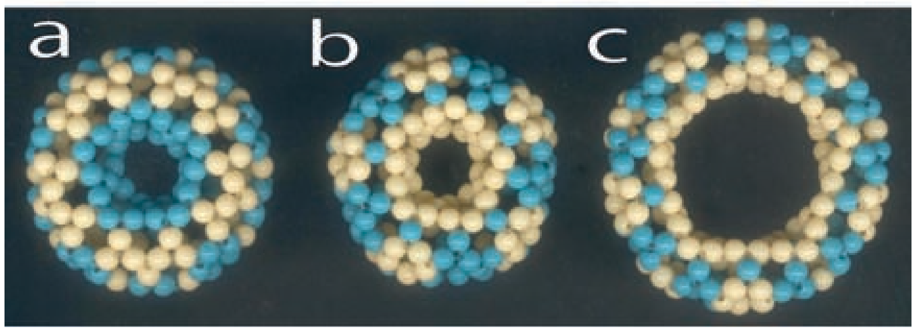


Stability

Rotational dependence of AM1 HOF of TCNTs with number of atoms less than 40 per unit cell.

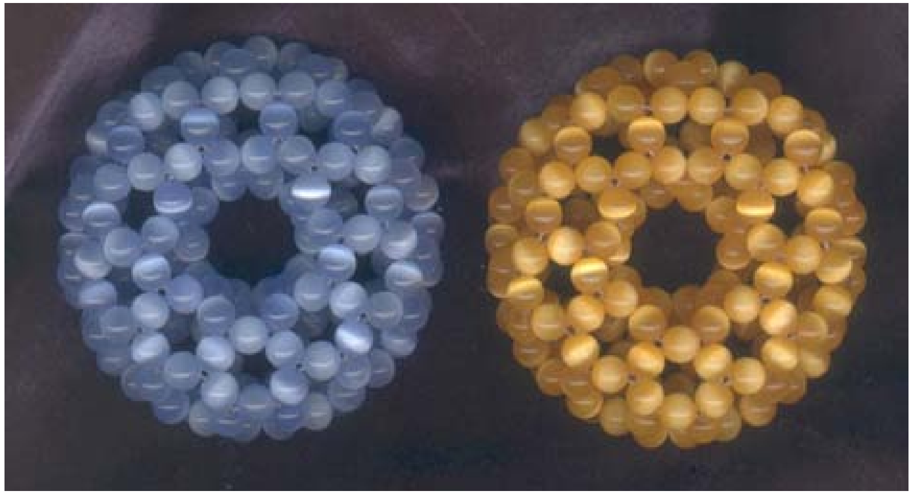


TCNTs with 120 atoms

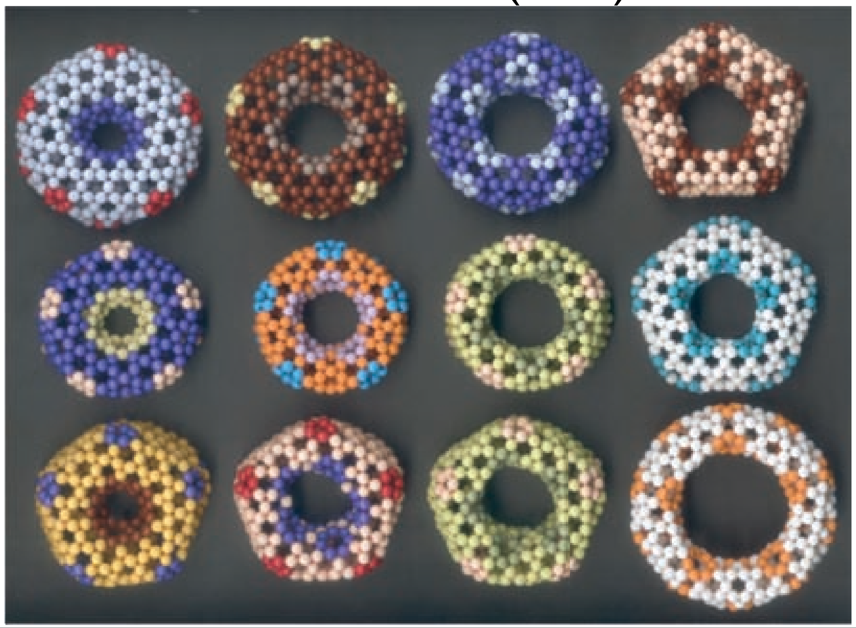


Key chain

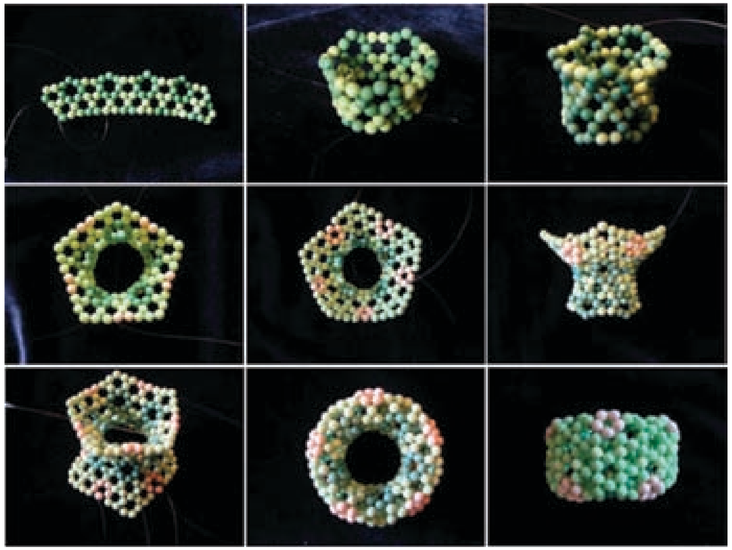
貓眼石串珠



TCNT 240 (T_{240})



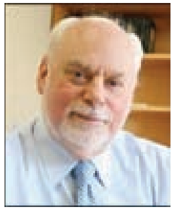
T_{240} 的製作過程



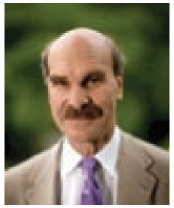
Synthetic attempts (Mar. 2011)

A. Gamburd (UCSC)

西北大學

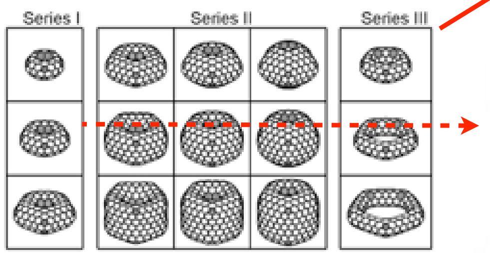


J. F. Stoddart

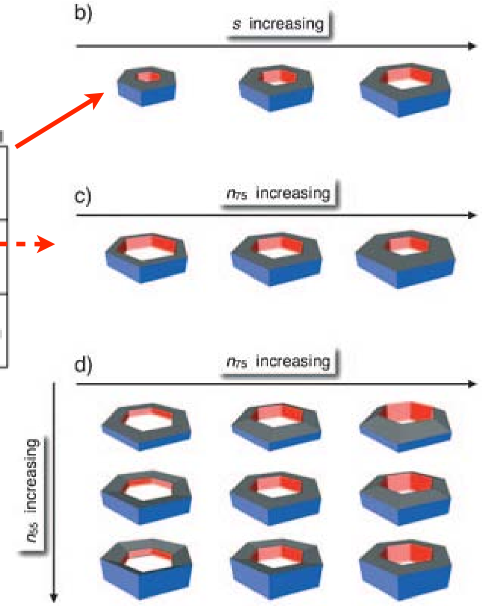


M. Ratner

Cover Picture: Optical and Vibrational Properties of Toroidal Carbon Nanotubes (Chem. Eur. J. 14/2011) F. Beuerle, C. Herrmann, A. C. Whalley, C. Valente, Alexander Gamburd, Mark A. Ratner, J. Fraser Stoddart

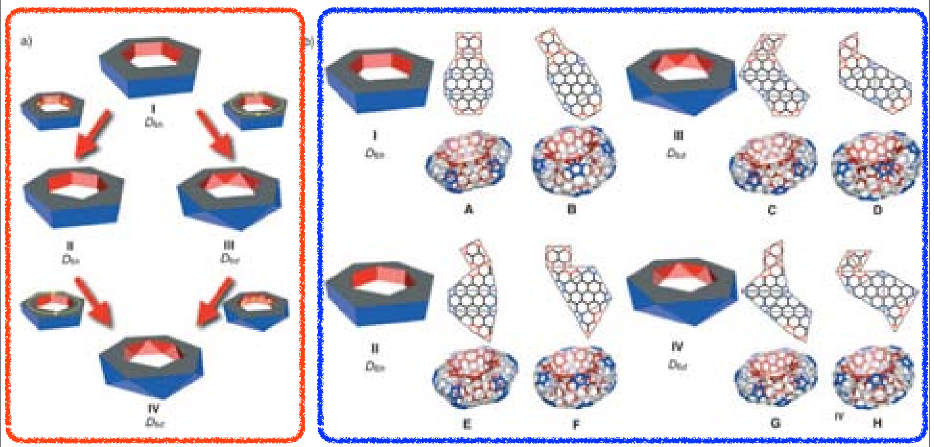


C. Chuang et al. *J. Chem. Inf. Model.* 2009, 49, 361-368

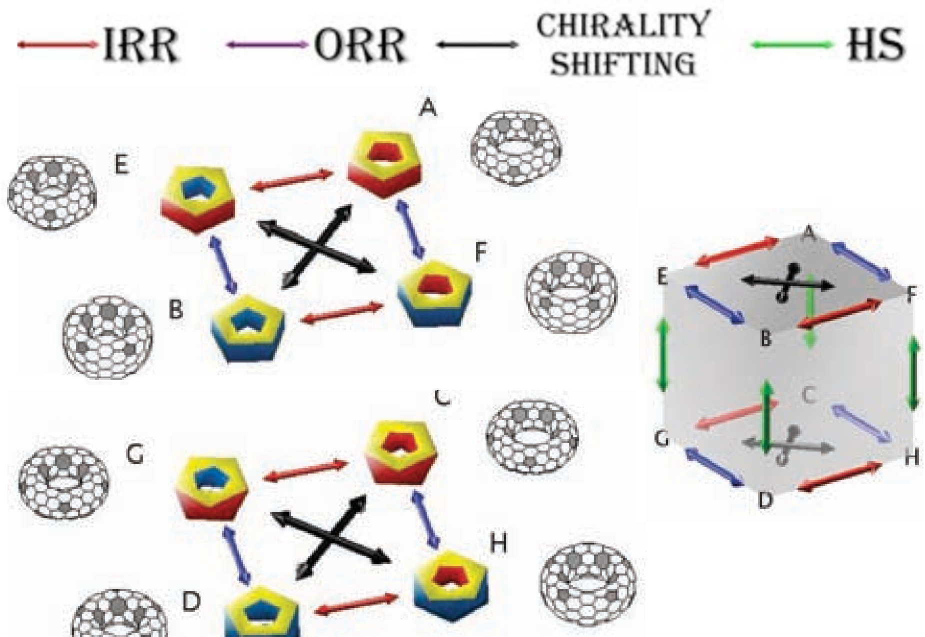


F. Beuerle et al *Chem. Eur. J.* 2011, 17, 3868-3875 (Mar. 2011)

Eight structural types identified by Beuerles et al.

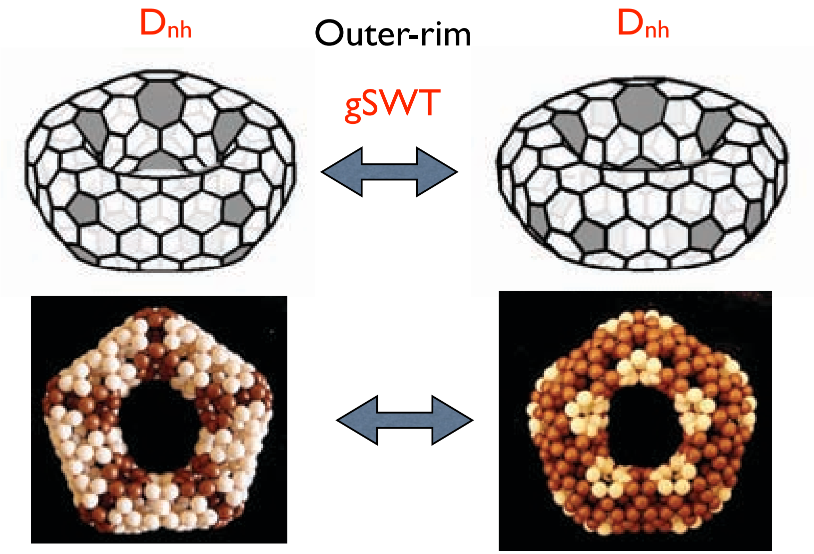


F. Beuerle et al *Chem. Eur. J.* 2011, 17, 3868-3875 (Mar. 2011)

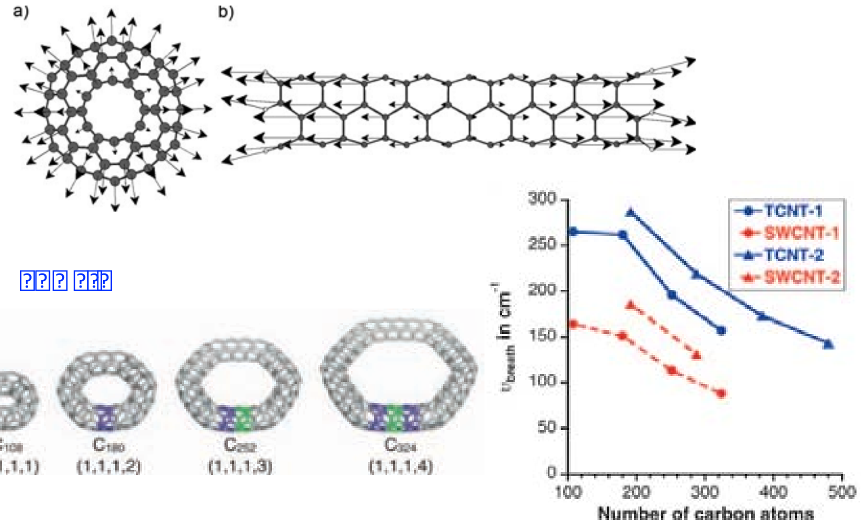


Chuang and Jin, *Comment on the structural types of TCNTs*, to be submitted to *Chem. Eur. J.*

Three extra types without latitudes

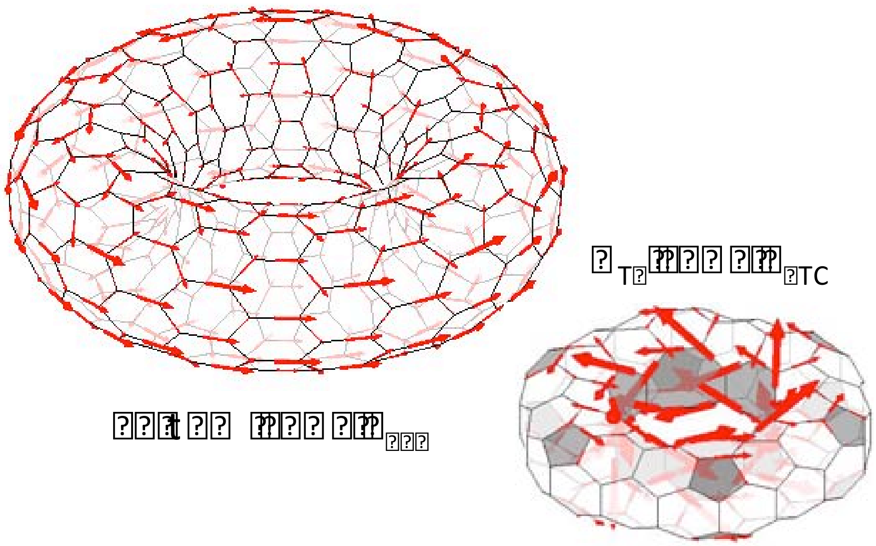


□□□u□□□□□□□□□et g□□□e□□□ □□2

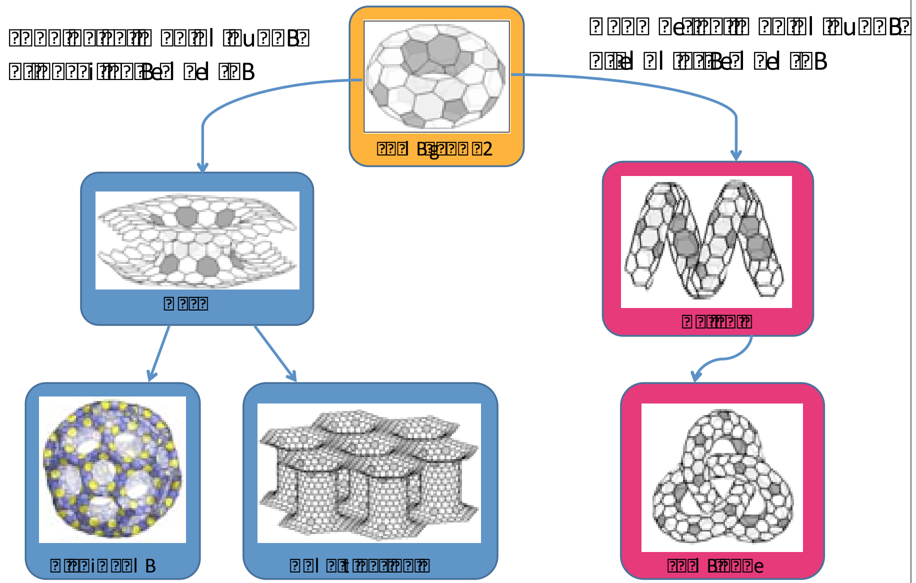


F. Beuerle et al *Chem. Eur. J.* 2011, 17, 3868-3875

□□□B□Be□□e□□l □□□□eB

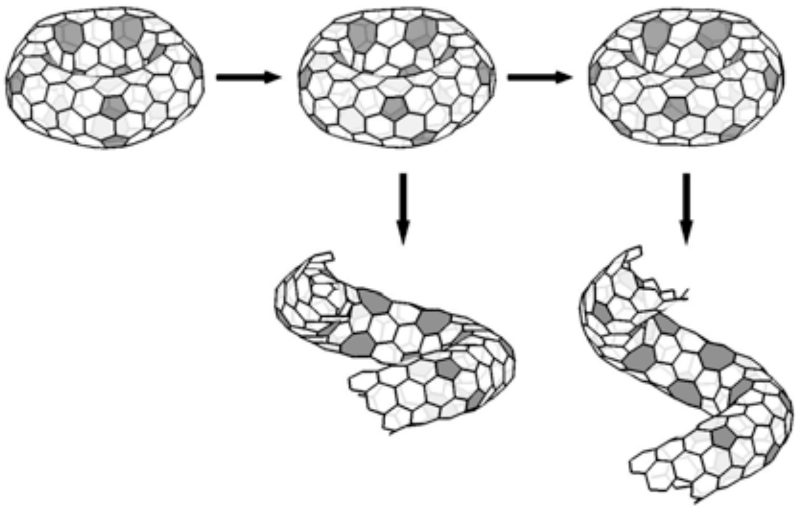


Hierarchy of Graphitic Structures



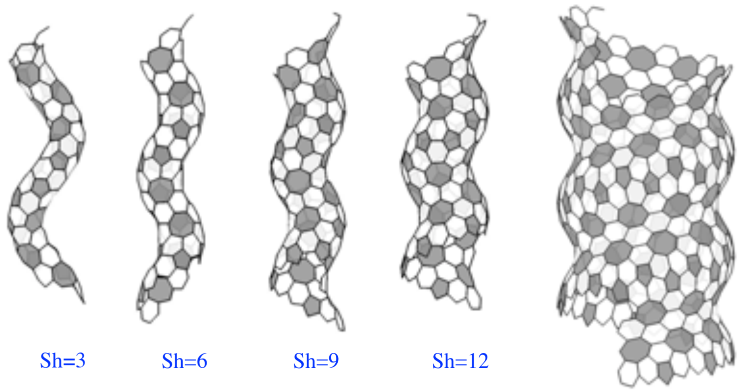
Helically Coiled CNT (HCCNT)

Coil Formation by Horizontal Shift



HCCNT and shifted parameter

All nonhexagons are separated by on CC bond.

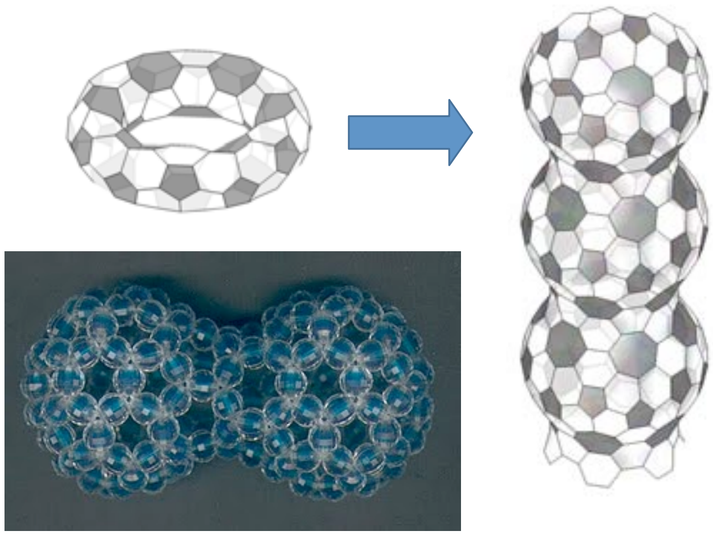


Sh=3 Sh=6 Sh=9 Sh=12 Sh=30

Buckyhelices of higher shifting parameter Sh.

Chuang, C; Jin, B.-Y.* Hypothetical toroidal, cylindrical, helical analogs of C_{60}
J. Mol. Graph. Model. **2009**, 28, 220-225.

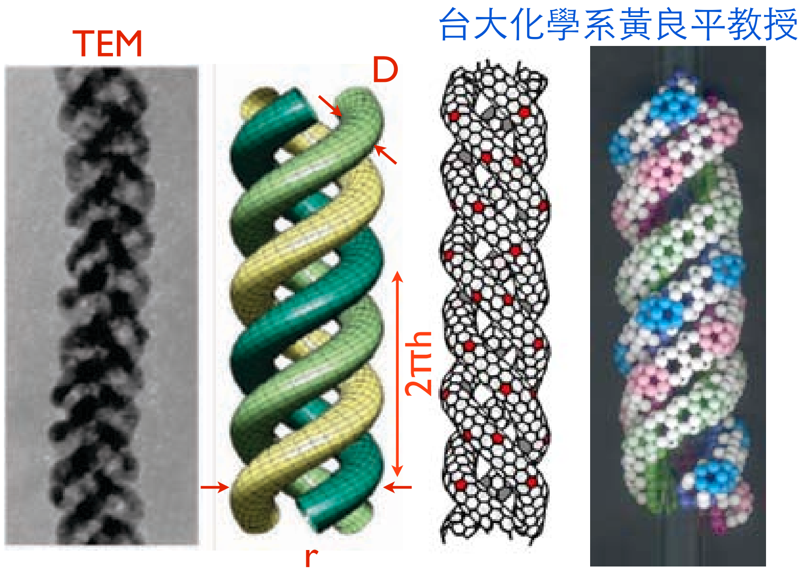
Buckled CNT Derived from TCNT



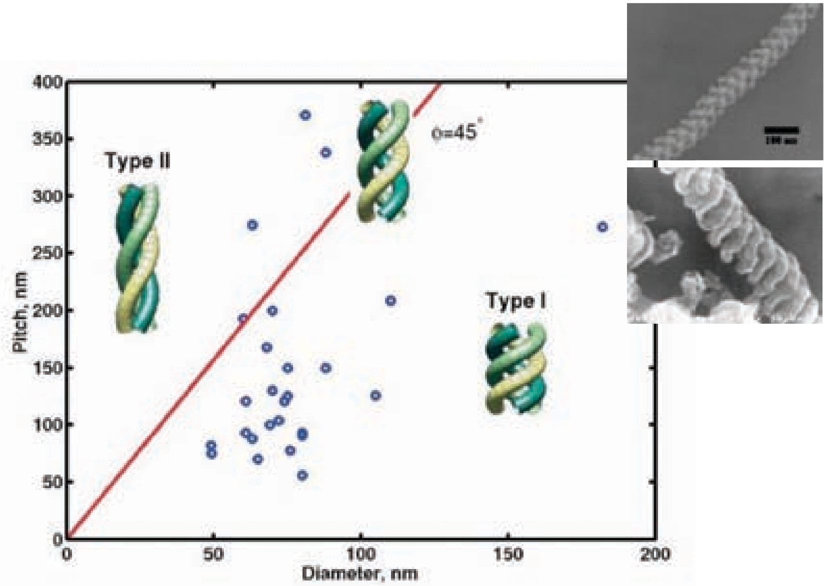
Helically Coiled CNT (HCCNT)

Helical Coiled Carbon Nanotube (HCNT)

Triple Stranded Carbon Helix

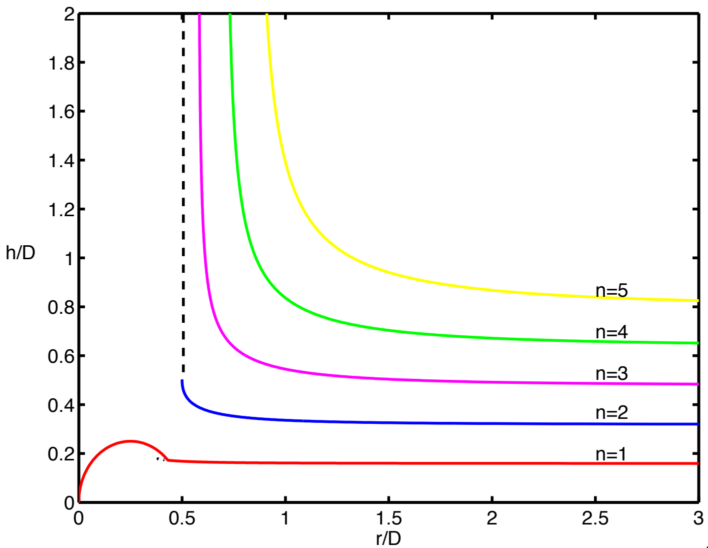


Su, C.-J.; Hwang, D. W.; Lin, S.-H.; Jin, B.-Y.*, Hwang, L.-P.* Self-organization of triple-stranded carbon nanoropes *Phys. Chem. Comm.* **2002**, 5, 34.



Su, C.-J.; Hwang, D. W.; Lin, S.-H.; Jin, B.-Y.*, Hwang, L.-P.* Self-organization of triple-stranded carbon nanoropes *Phys. Chem. Comm.* **2002**, 5, 34.

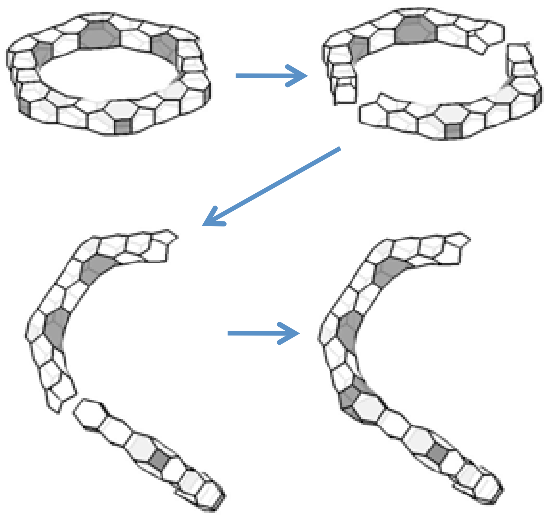
Phase diagram



楊定學

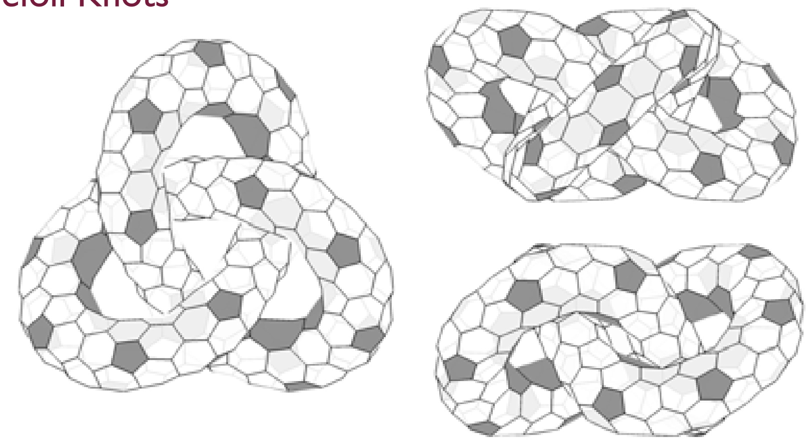
Vertical Shifting

Helicity of 2nd Kind

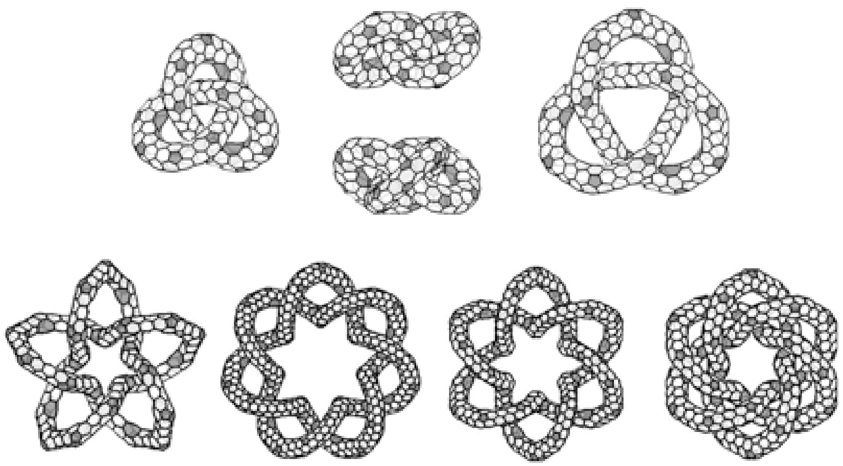


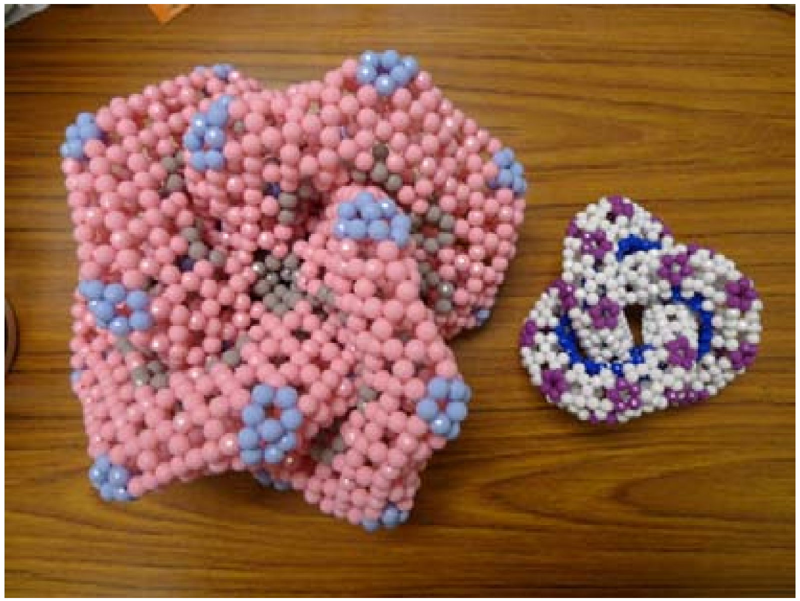
Combination of Two Kinds of Helicities: CNT Space Curves

Trefoil Knots



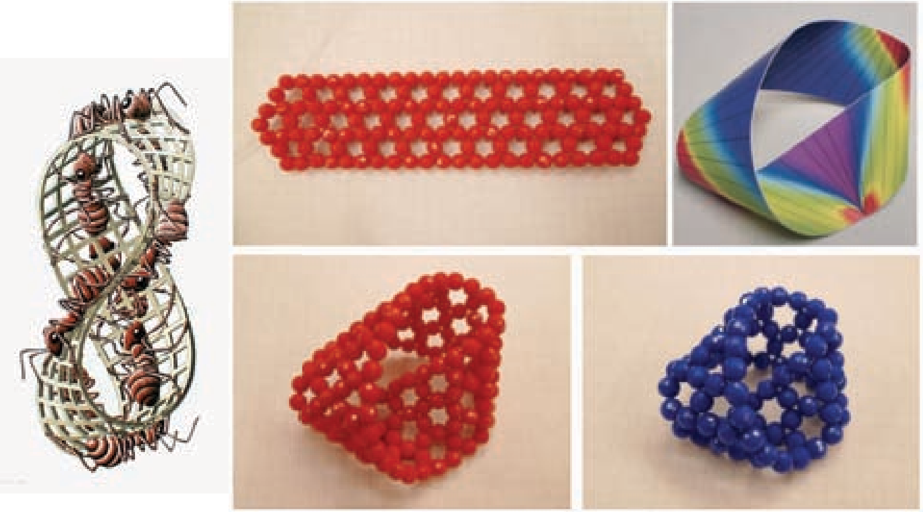
[illegible]



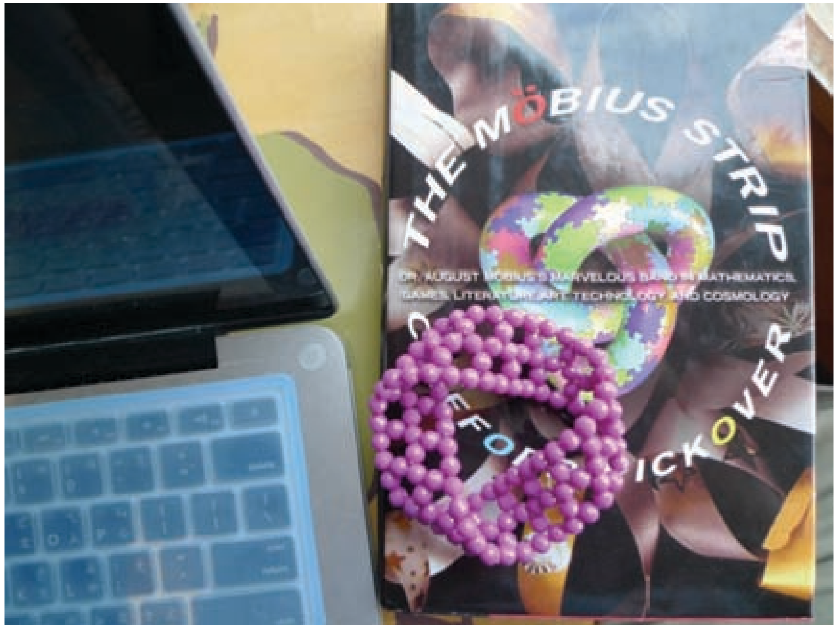


黃千睿

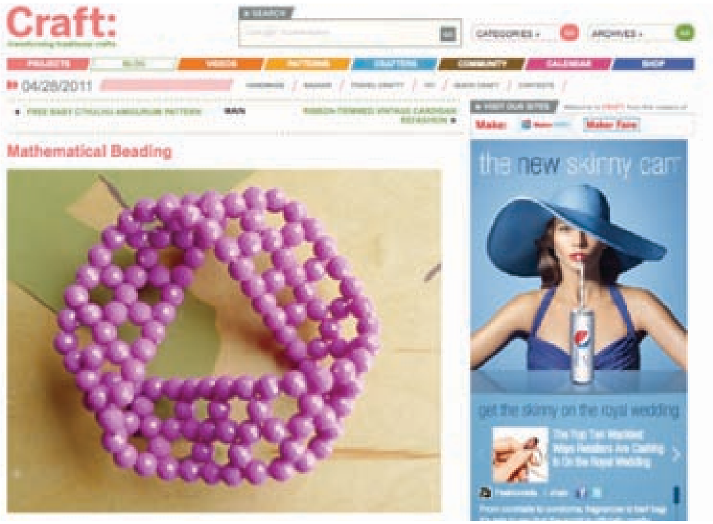
Möbius Band



E. L. Starostin, G. H. M. van der Heijden, The shape of Möbius strip, Nature materials, 6. 563 (2007).



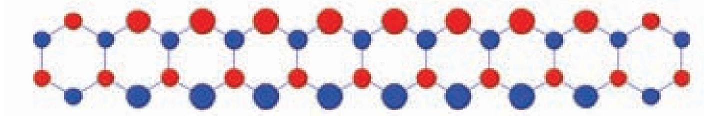
Craft magazine



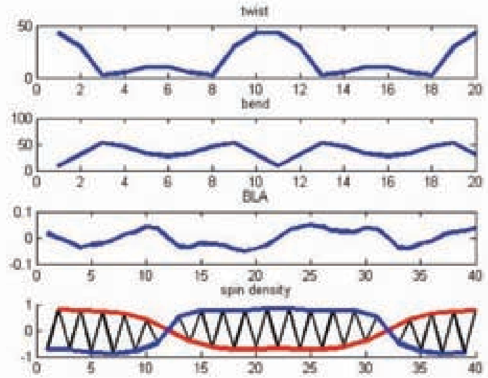
Crafts and science (or the science of crafts?)

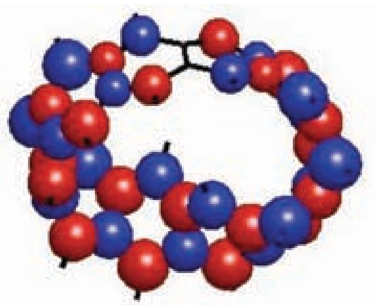
http://blog.craftzine.com/archive/2010/06/mathematical_beading.html

Spin solitons in Möbius carbon nanoribbons with zigzag edge

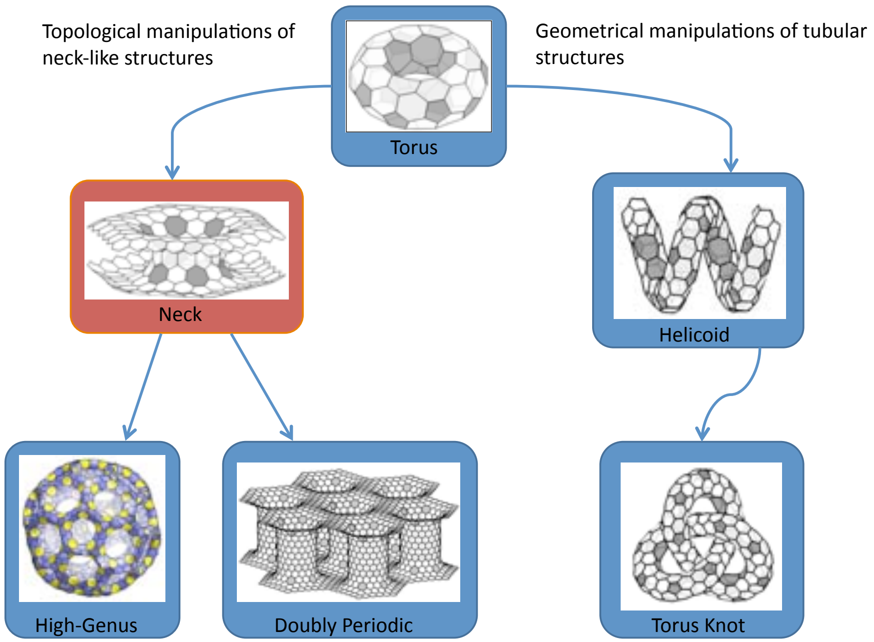


Spin density in polyacene

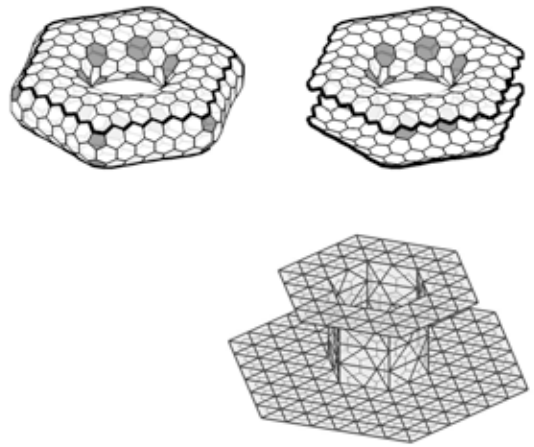


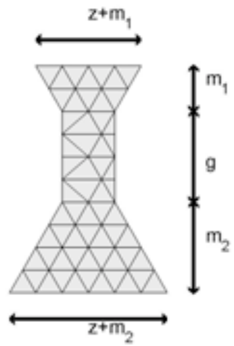


許睿玄



Neck Structure: Construction of High Genus Fullerenes

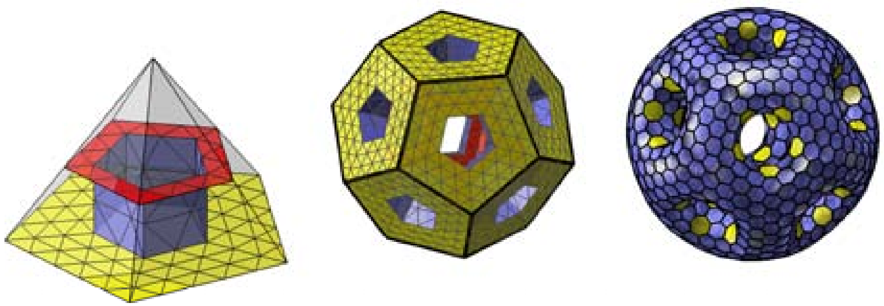




Chuang & Jin, J.Chem.Inf & Model 2009

High Genus Fullerenes

Dodecahedron (genus 11)

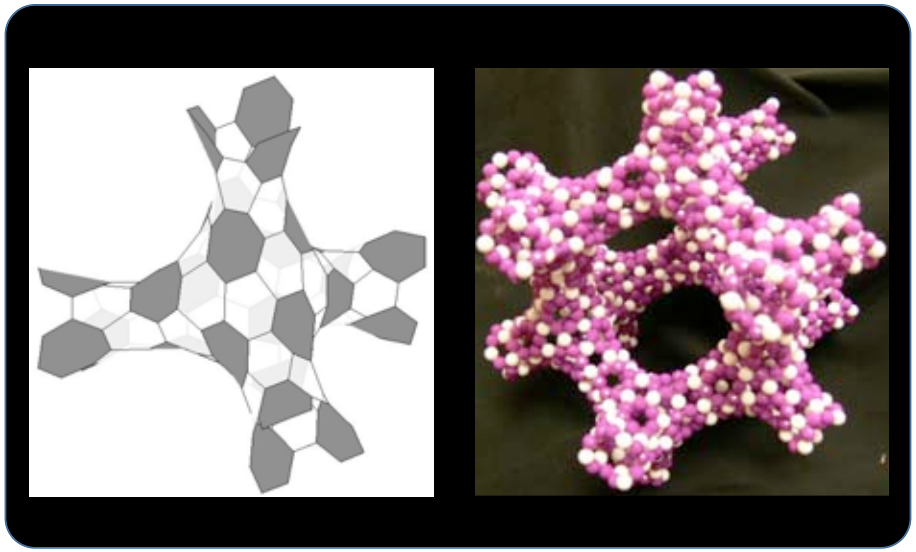


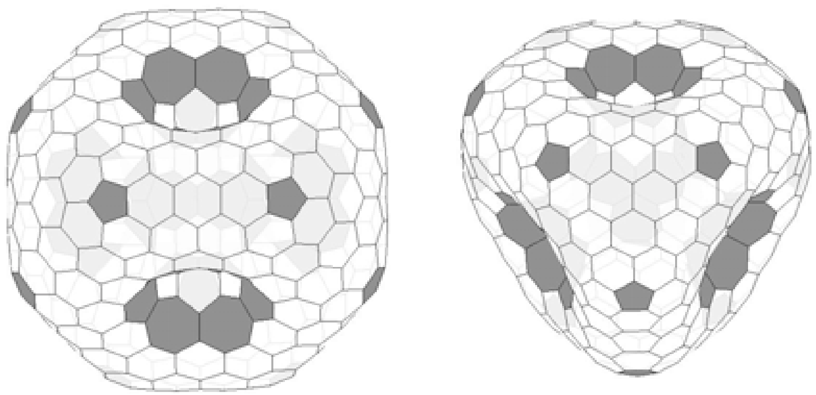
This kind of structures is originally proposed by H.Terrone and A. Mackay.

Chuang, C; Jin, B.-Y.* Systematics of High-Genus Fullerenes *J. Chem. Info. Model.* **2009**, 49, 1664-1668.

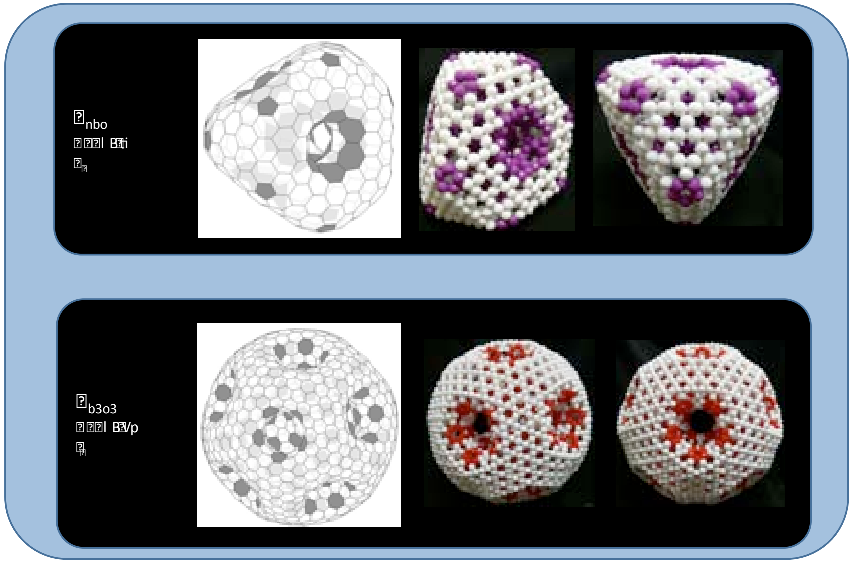
李文卿教授

C_{168}

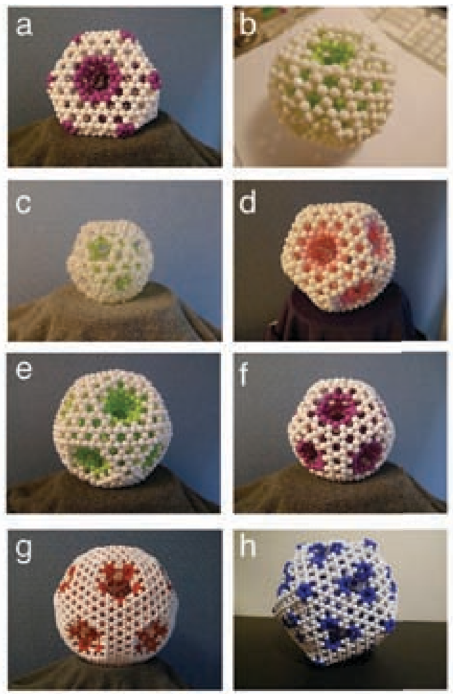




串珠模型：高虧格芙類芙類分子

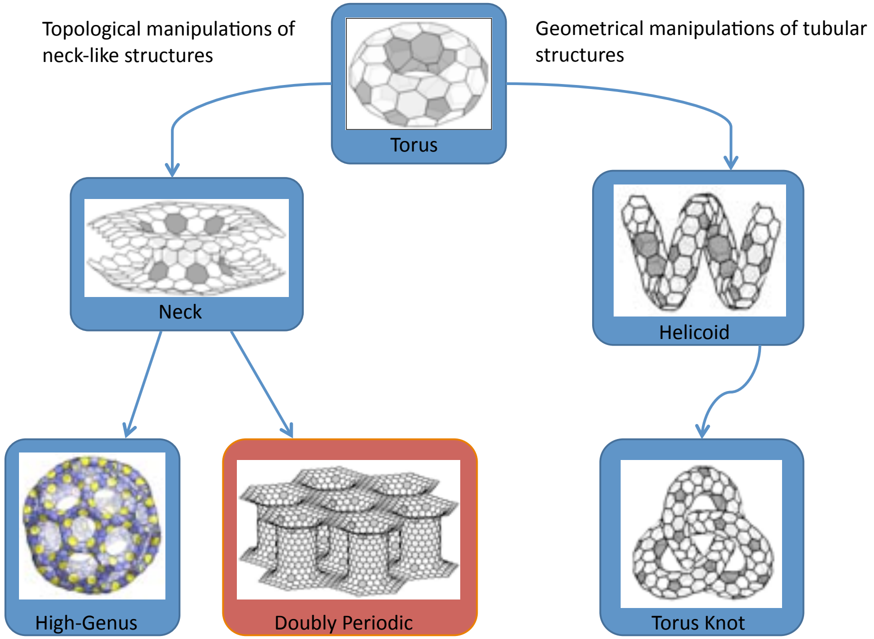


Chuang, C.; Jin, B.-Y.; Tsoo, C.-C. Designing Sculptures Inspired by High-Genus Fullerenes with Mathematical Beading *Proceedings of Bridges: Mathematical Connections in Art, Music, and Science*, **2011**. accepted

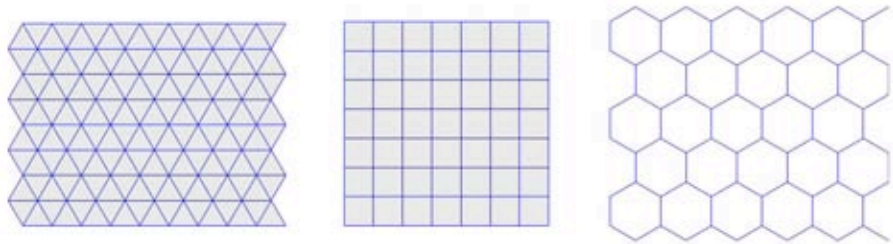


Metabolic Sphere

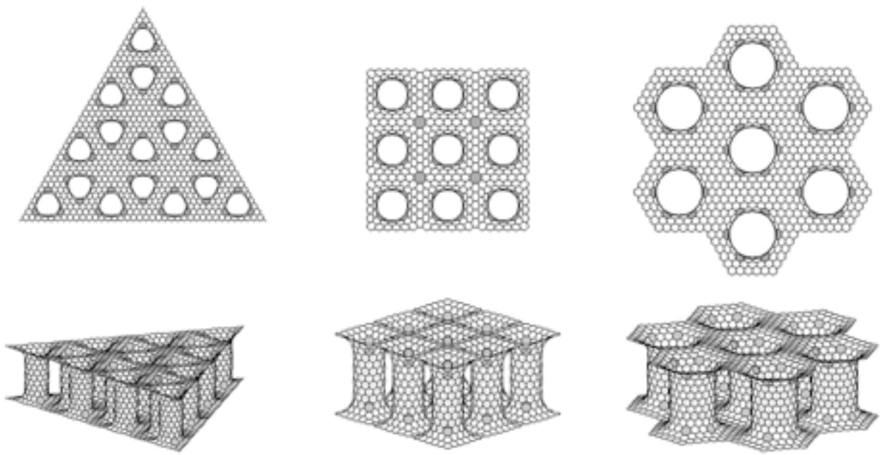
Presented as part of Nobel Textiles in St James Park, London for the London Design Festival 2008.



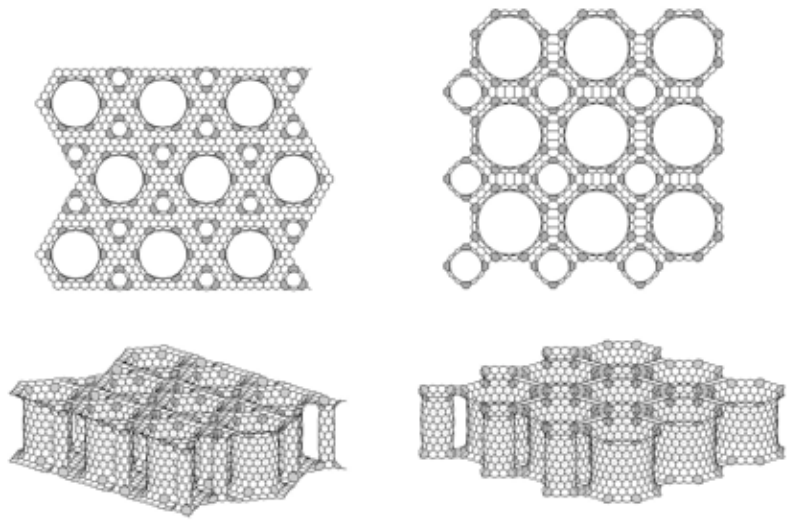
Platonic tilings



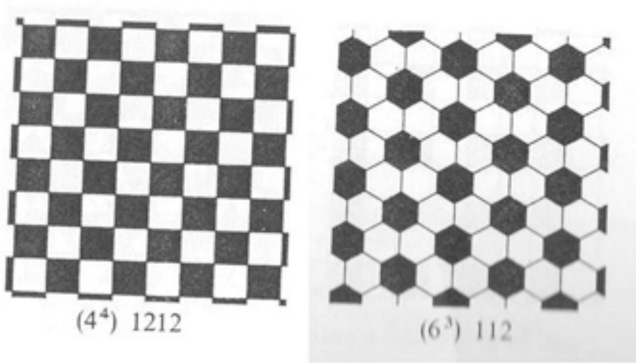
Neck Structure on Platonic Tiling



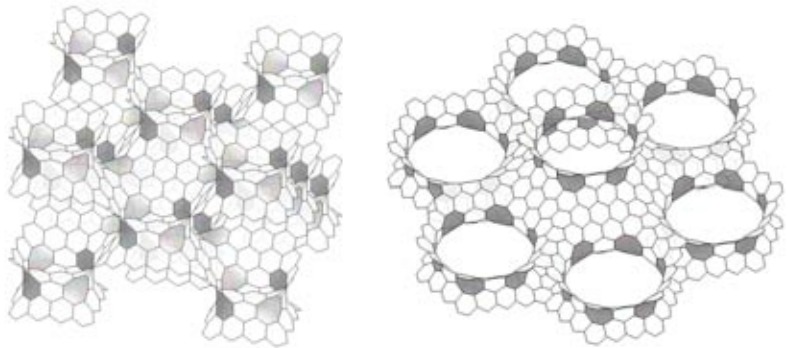
Neck Structure on Archimedean Tiling



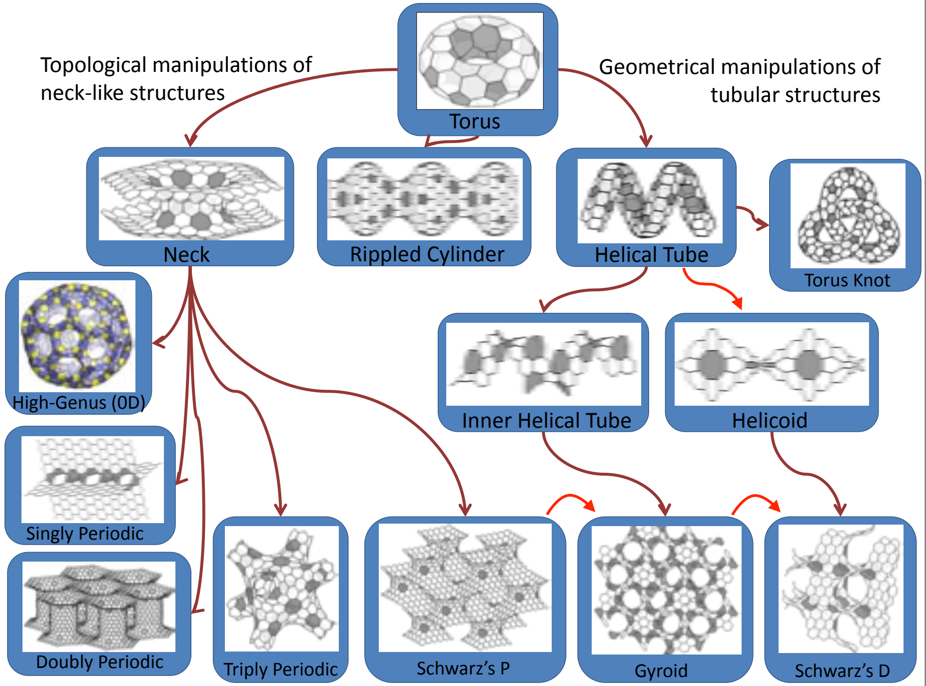
Colored Regular Tilings



Triply Periodic Structures from Colored Regular Tilings

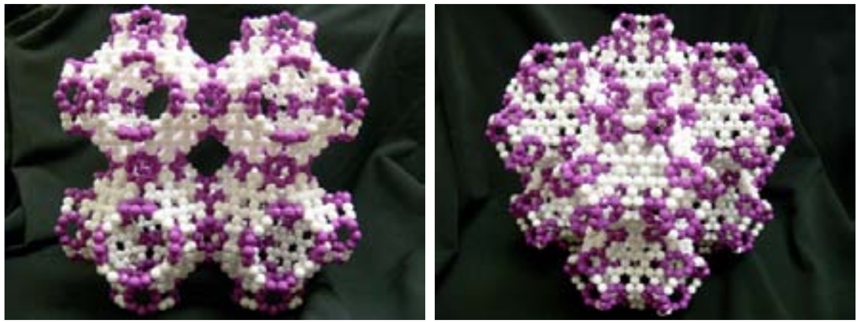


Schwarz's P surface



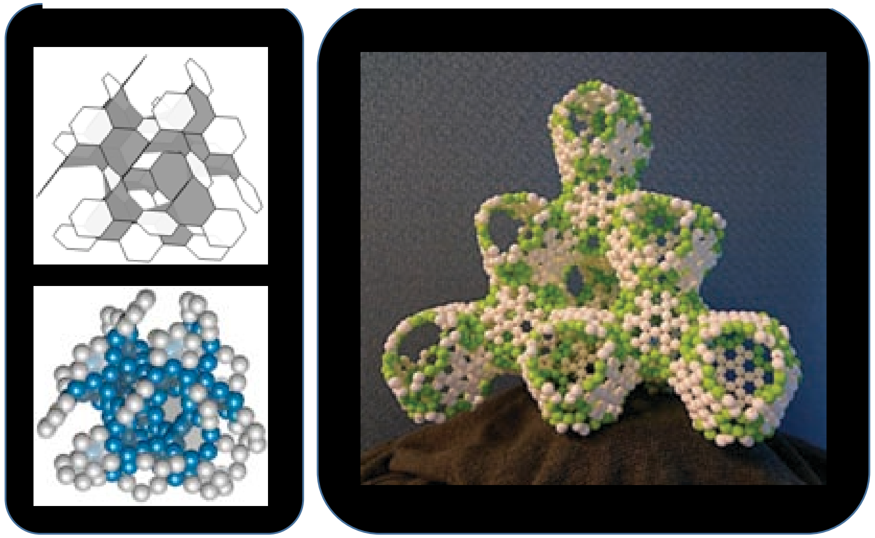
Triply Infinite Periodic Minimal Surface

P-型最小曲面



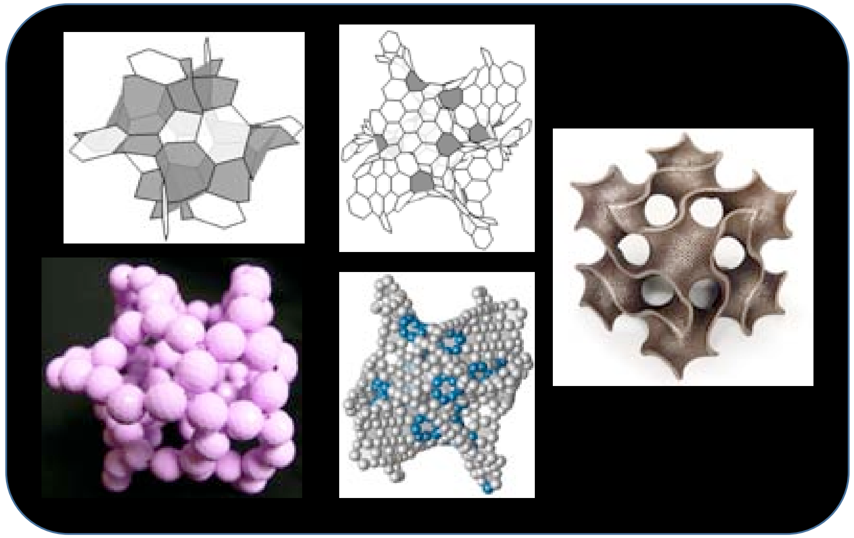
Jin, B.-Y.*; Chuang, C.; Tsoo, C.-C. Constructing Molecules with Beads: The Geometry of Topologically Nontrivial Fullerenes *Proceedings of Bridges: Mathematical Connections in Art, Music, and Science*, **2010**, 391-394.

D-型週期最小曲面



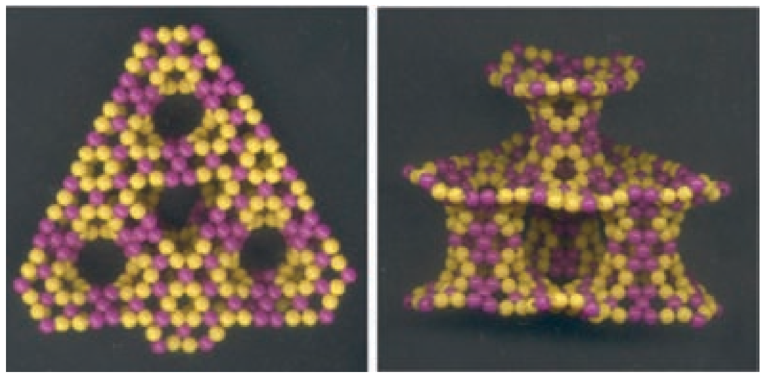
魏緯齊

螺旋型最小曲面（G-型）

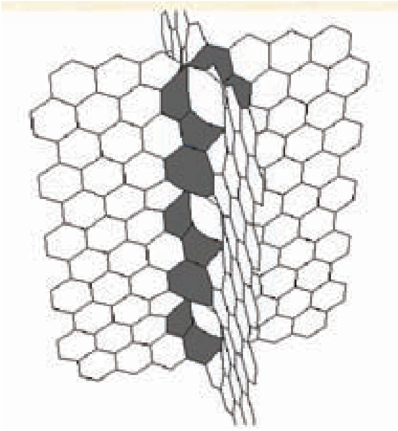


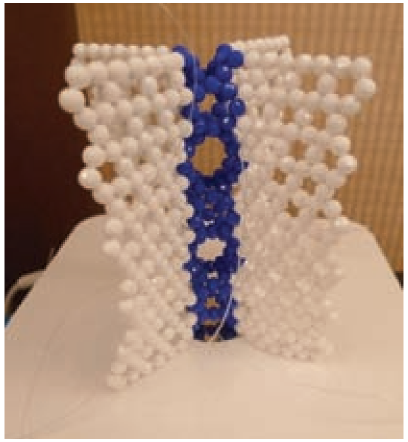
Graphitic gyroid

H-型曲面

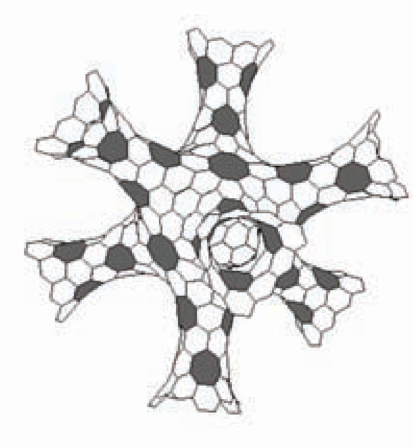


Scherk Singly Periodic Minimal surface



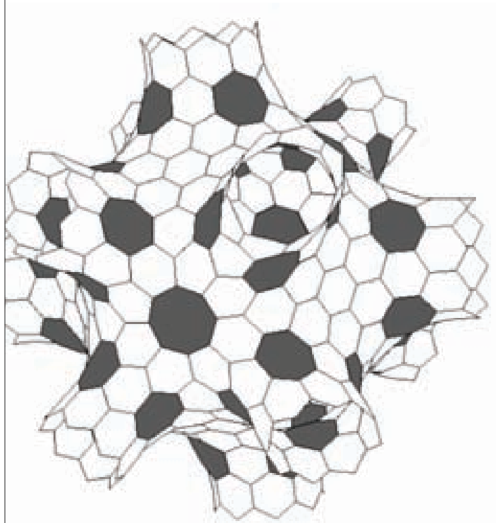


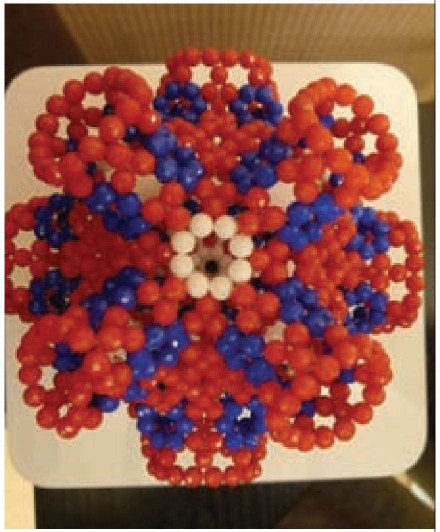
Schoen's IWP Surface



Schoen's IWP Surface (2x2x2)

Nevious surface





Sierpinski buckyball

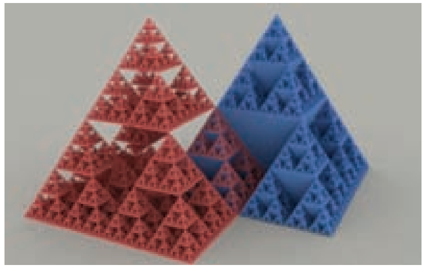
Hausdorff (fractal) dimension

$D = \log 90 / \log$ scaling factor

$= \log(90)/\log(7) \sim \log(90)/\log(6.5)$

$= 2.3 \sim 2.4$

Sierpinski's pyramid



http://commons.wikimedia.org/wiki/Image:Sierpinski_pyramid.png

THE BEADING GEM'S JOURNAL

Jewelry Expressions in Bloom

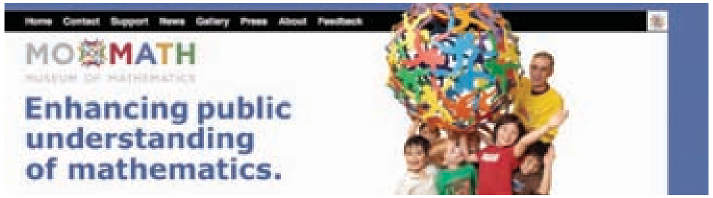
SUNDAY, MAY 23, 2010

Beaded Fullerenes : 3D Molecular Structures

Tweet Like 1K

Virtually all the tutorials I have featured on this blog have come from other jewelry artisans or crafters. So for the first time (not counting myself), I am featuring how-tos from scientists, specifically the Chemistry Department of the National Taiwan University!

How did that happen? Well, they make beaded models of a type of carbon molecule called



Math Monday: Mathematical Beading

JUNE 7, 2010

by George Hart

Beading is a traditional craft which recently has been applied to make interesting mathematical models. Here are some impressive examples by Bih-Yaw Jin, starting with a beaded Mobius strip.

http://momath.org/home/math-monday-06-07-10/

Carnival of Mathematics

Issue 67, 2 July 2010 | Travels in a Mathematical World | 67¢

Culture

At the Make: Online blog, George Hart, for the Museum of Mathematics, writes a Math Monday article on Mathematical beading. This includes the image above - can you tell what it is? Go to the article to find out. George gives five examples by Bih-Yaw Jin, and asks What interesting shapes can you make with beads?

http://travelsinamathematicalworld.blogspot.com/2010/07/carnival-of-mathematics-67.html

“CASE □ Center for the Advancement of Science Education
□□ □ □□□□□□□□□□□□□□”

【科學工藝】化學家用珠珠串出富勒烯（Fullerene）家族

• 從前從前，有一個化學家經過手工材料行林立的延平北路，看見了櫥窗裡有些閃閃發光的奇妙東西。「我忽然發現，咦！這些東西怎麼長得好像…芙類分子？」這就是台大化學系金必耀教授與串珠的相遇過程。

http://case.ntu.edu.tw/blog/?p=3550

緣起：小熊媽媽

延平北路

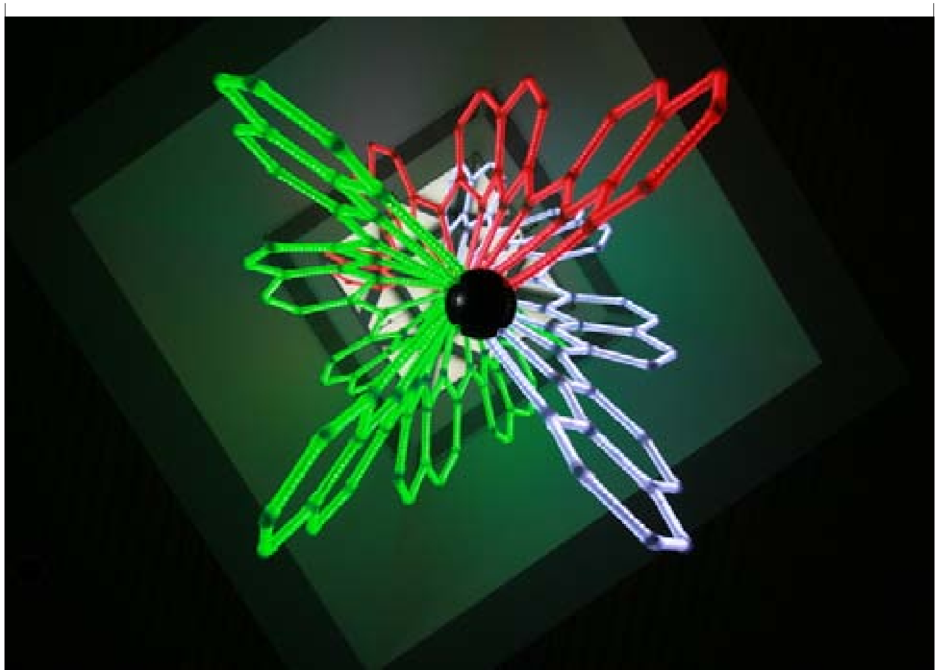
櫥窗一景


台灣大學化學系
2005年第一期工程 (北館)完工
2009年第二期工程
(積學館/南館)完工
劉勰 文心雕龍:「積學以儲寶、酌理以富才」

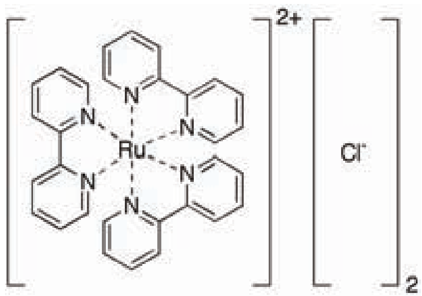

台大化學系
原分所
醉月湖與化學館之鳥瞰圖


醉月湖與化學館之夜景


彭旭明教授的
金屬串分子



The longest metal string reported to date for a single molecule comprises 11 nickel atoms. The mixed-valent Ni^{I} and Ni^{II} centers are arranged linearly and wrapped by four helical ligands. Flanking the molecular structure are images of the real molecular model that is on display in the Chemistry Building at the National Taiwan University, where the compound was designed and prepared. In their Communication on page 2045 ff. M. Bénard, S.-M. Peng, and co-workers also report the electronic and magnetic properties of this Ni_{11} complex.

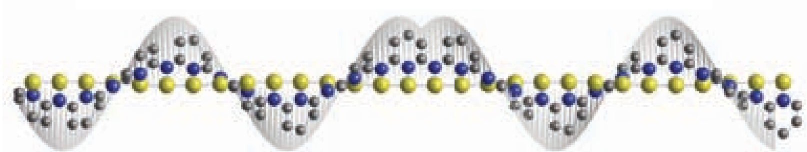


d^2sp^3 hybridization

黃千睿

Physical modeling through mathematical beading

Helical soliton excitation should be energetically possible.



Hopefully, temperature dependent NMR can prove this prediction by mathematical beading.

Wonder How To

http://www.wonderhowto.com/wonderment/mathematical-beading-accessories-thought-0116915/

Mathematical Beading: Accessories to Thought

How-To Topics » beaded fullerenes, Bih Yaw Jin, Mathematical Beading

1,807 views SHARE COMMENTS (0) HISTORY

Subscribe to the Wonderment RSS Feed or get Email Updates

Started By getexcellent

Published last month

Math is unreasonably effective in describing the natural universe. Anyone who's seen Walt Disney's *Donald in Mathmagic Land* knows this to be so. Well, the axiom works in reverse, too: The physical stuff of the universe can model math right back. And to great effect.

For proof, look no further than these beautiful beaded fullerenes crafted by Taiwanese chemistry professor Bih-Yaw Jin.

Thank You for your attention!

"Principles for the Development of a Complete Mind:

Study the science of art.

Study the art of science.

Develop your senses - especially learn how to see.

Realize that everything connects to everything else."

Leonardo da Vinci