Constructing Molecules with Beads: The Geometry of Topologically Nontrivial Fullerenes

Bih-Yaw Jin[a], Chern Chuang[a] and Chia-Chin Tsoo[b]
[a]Department of Chemistry, Center of Theoretical Sciences, and Center of Quantum Science and Engineering, National Taiwan University, Taipei, Taiwan, ROC
[b]National Center for High-Performance Computing, Hsin-Chu, Taiwan, ROC
E-mail: byjin@ntu.edu.tw

Abstract

Three-dimensional molecular structures of topologically nontrivial fullerenes (consisting of either finite or extended structures) are usually aesthetically pleasing. In this article, we demonstrate that beads such as the ones commonly used in decorative art and ornament making can also be used to construct arbitrary fullerene structures. Based on the spiral codes of fullerenes, we developed a systematic strategy for making physical models of cage-like fullerenes use common beads. The resulting beaded model structure is similar to the true three-dimensional molecular structure of corresponding fullerene due to an interesting analogy between the hard-sphere repulsion among neighboring beads and the microscopic valence shell electron pair repulsion for the sp^2-hybridized carbon atoms. More complicated fullerenes models that have nontrivial topology (e.g. toroidal carbon nanotubes, helically coiled carbon nanotubes, and high-genus fullerenes) can also be faithfully constructed using beads. Beaded models of extended graphitic structures such as those that correspond to tiling of graphene sheet on a Schwartz P- and D-surfaces, Shoen I-WP, and Nervious surfaces, can also been created.

Physical models of molecular systems are indispensable in understanding the three-dimensional molecular shapes of complicated 3D molecular structures. The relationships among the various parts of molecules become more transparent with a physical model in hand. There are many different ways to construct a physical model of a molecular system. Usually an explicit representation of atoms is adopted. This is the case for most commercial molecular model sets in which the standard ball-and-stick model is used to construct small organic or inorganic molecules. In this article, we will demonstrate that beads such as those commonly used in ornaments, crafts, and decorative art can be used as a versatile, low-cost, high-quality material for creating faithful three-dimensional structures of carbon nanostructures with positive or negative Gaussian curvatures.[1] The application of "beading" to molecular modeling has been proven useful in helping to visualize the geometrical structure of complex carbon nanomaterials.

The beaded fullerenes, as shown in Fig. 1, is not only aesthetically pleasing to look at, but the resulting shapes are consistent with the optimized geometries based on more sophisticated molecular force fields in the most important structural features. The reason for this agreement is not a coincidence; rather, it arises out of the mechanical interactions in the beaded molecules and the steric repulsion in the sp^2-hybridized fullerenes. The geometry of the beaded molecules is determined primarily by the steric repulsion between the beads themselves, this being a simple macroscopic realization of the Valence-Shell Electron-Pair Repulsion theory. The beaded models are, thus, a bond-representation of fullerenes as opposed to the more commonly seen atom-representation of traditional ball-and-stick models. It is, therefore, advantageous to have a beaded model since its actual physical shape can actually be felt when touching it and a mechanical response can be observed when it is pressed upon. Additionally, the influence of the spatial arrangement of the five- and seven-membered rings on the three-dimensional structures of carbon nanotori is vividly displayed in the beaded fullerenes (Fig. 1b-e).

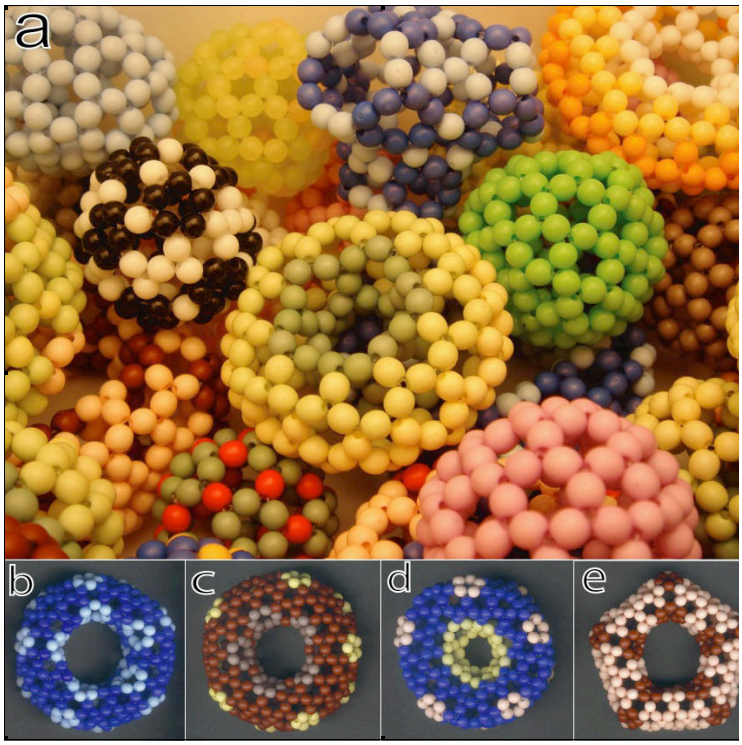

Figure 1: *Assorted beaded fullerenes (a) and four toroidal carbon nanotubes (b-e).*

We also discovered that all the information needed to weave a beaded fullerene is contained in the spiral code, which is now enshrined in the IUPAC nomenclature of the molecule[2]. Based on the prescribed spiral code, the physical model of a fullerene can be constructed by stitching the beads together with a long nylon thread using the so-called Right Angle Weave (RAW) technique. Since the procedure for beading a fullerene consists of nothing more than repeating the RAW technique to generate a sequence of five-, six-, and seven-bead groups, we only needed the specification of the arrangement of polygons in a fullerene in terms of the linear sequence of numerals, which is equivalent to the Fowler's spiral algorithm[3].

The minimum length of nylon thread needed to weave the beads together corresponds to the Hamiltonian circuit problem in mathematics. According to the spiral code, each bead is stitched twice to create a fullerene, therefore, the length of the thread needed should be approximately twice the number of beads used, 2Nd. The actual length of thread needed for stitching can be determined using a scaling factor given by the ratio of the actual length of thread used in building the molecule and the corresponding minimum length, s=L/2Nd. By performing a few measurements on the length used to weave the beaded models, we determined the scaling factor to be about 1.1~1.2. Including the extra length required for tightening up the final beaded molecule (about K=20 to 30 cm), the formula for the total length of thread needed to build a fullerene with M carbon atoms is L=3sMd+K. We had to stitch through several beads more than twice when beading the fullerene without a spiral.

In principle, common beads can be used to construct any simple fullerenes with cage-like shapes (genus=0) as well as other more complicated structures such as toroidal shapes[4] (genus=1, Fig. 1b-e), helically coiled carbon nanotubes[5] and torus knots (Fig. 2), singly-, doubly- and triply-periodic minimal surfaces[6] (Fig. 3), high-genus fullerenes[7] (Fig. 4), Sierpinski buckyballs (Fig. 5), and Möbius bands. Below are some beaded models containing more complicated geometries that we constructed over the last few years.[8,9]

Helically coiled and torus knot carbon nanotubes.

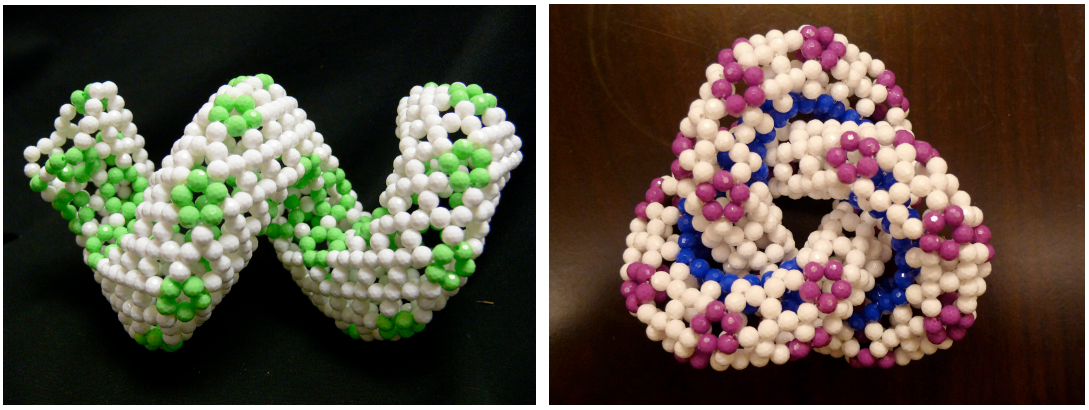

Figure 2: *Beaded model of the helically coiled carbon nanotube and the trefoil knot carbon nanotube.*

Graphitic Structures with Negative Gaussian Curvatures.

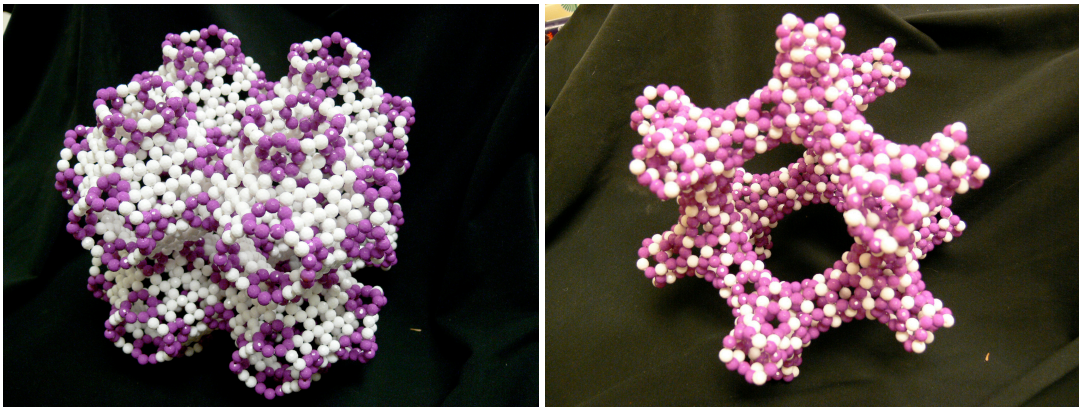

Figure 3: *Beaded models of P-type triply periodic minimal surfaces and C_{168} in the hyperbolic space.*

High-genus fullerenes.

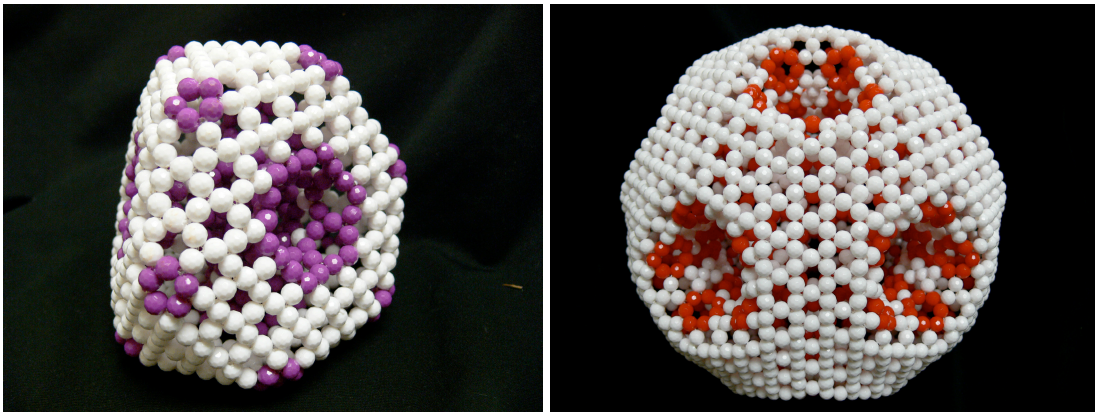

Figure 4: *Beaded models of high-genus fullerenes.*

Sierpinski buckyball.

Figure 5 :*Beaded model of the Sierpinski buckyball.*

In conclusion, we demonstrated that beads can be used as a generic material to successfully construct faithful three-dimensional models of arbitrary fullerenes. There are many advantages to using beads over traditional modeling methods. Robust physical models of complicated carbon nanostructures with sp^2 hybridization can be created more easily and economically using beads rather than other methods.

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References

[1] Bih-Yaw Jin, Chern Chuang, Chia-Chin Tsoo, *The Wonderful World of Beaded Molecules* (in Chinese), Chemistry (Taipei), Vol. 12, pp. 19-25. 2008.
[2] E. W. Godly, R. Taylor, *Nomenclature and terminology of fullerenes: A preliminary study*, Pure Appl. Chem. Vol. 69, pp. 1411-1434 (1997).
[3] P. W. Fowler, D. E. Manolopoulos, *An Atlas of Fullerenes*, (Oxford University Press, 1995).
[4] Chern Chuang, Yuan-Chia Fan, Bih-Yaw Jin *Generalized Classification of Toroidal and Helical Carbon Nanotubes*, J. Chem. Info. Model. Vol. 49, pp. 361-368, 2009.
[5] Chern Chuang, Bih-Yaw Jin, *Hypothetical toroidal, cylindrical, helical analogs of C_{60}*, J. Mol. Graph. Model. Vol. 28, pp. 220-225, 2009.

[6] Chern Chuang, Bih-Yaw Jin, *Classification of Hypothetical Doubly and Triply Periodic Porous Graphitic Structures by Tilings of Neck-Like Units*, J. Math. Chem. Vol. 47, pp. 1077, 2010.

[7] Chern Chuang, Bih-Yaw Jin, *Systematics of High-Genus Fullerenes*, J. Chem. Info. Model. Vol. 49, pp. 1664-1668, 2009.
[8] An extensive list of beaded models of many different types of fullerenes can be found at http://thebeadedmolecules.blogspot.com.
[9] Constructing a beaded model is a slow sequential process. It takes an experienced beader about 30 minutes to make a C_{60}. More than 20 working hours are needed to construct a more complicated graphitic structure such as a 2x2x2 P-type periodic minimal surface as shown in Fig. 3.