Designing Sculptures Inspired by Symmetric High-Genus Fullerenes with Mathematical Beading

Chern Chuang^a, Bih-Yaw Jin^a and Chia-Chin Tsoo^b ^aDepartment of Chemistry, Center of Theoretical Sciences, and Center of Quantum Science and Engineering, National Taiwan University, Taipei, Taiwan, ROC

^bNational Center for High-Performance Computing, Hsin-Chu, Taiwan, ROC E-mail: byjin@ntu.edu.tw

Abstract

We present a scenario of building beautiful sculptures inspired by high-genus molecules utilizing traditional beading techniques. These hypothetical molecules are highly symmetric trivalent fullerenes composed of hundreds of exclusively sp²-hybridized carbon atoms, with multiple handles. We describe the construction rules governing the structural features of the sculptures, which are basically two-layer regular polyhedra connected through straight tubules. Readers can follow the instructions to construct their own sculptures. The resulting beaded structures elegantly and faithfully reflect the geometry of the molecules obtained by sophisticated computer modeling approach, which themselves form a beautiful display of communication between science and art.

Introduction

Previously we have presented general aspects of constructing molecules, especially fullerenes, with beads used in traditional handmade jewelry [1,2]. Using the standard weaving technique commonly called the figure eight stitch in the oriental countries or the right angle weave in the west, one can create the physical models of arbitrary fullerenes faithfully. Here we proceed to elaborate that mathematical beading can be extremely helpful to the understanding of three-dimensional structures of complex molecules. Molecules having complex topology and geometry are often difficult to recognize and imagine. With physical models at hand we can largely reduce this difficulty. In addition, these bead models are attractive and aesthetically pleasing on their own and can be statically displayed as well.

We present the detailed construction scheme of high-genus molecules. These molecules, typically containing hundreds of atoms, are both of chemical interest and can serve as educational examples for geometry or topology. Readers can easily follow these construction rules to build their own zoo of beautiful sculptures with beads.

High-Genus Fullerenes: Cube as an Example

High-genus fullerenes can be theoretically constructed by assembling identical neck-like structures onto the faces of regular polyhedra. For the sake of simplicity, we take the cube as an example, which is the most familiar one, to general audience, among the five Platonic polyhedra. High-genus fullerenes corresponding the other four Platonic solids can be achieved in similar fashion.

Starting with a fourfold rotational symmetric toroidal carbon nanotube, as shown in Figure 1(a). A stable toroidal carbon nanotube is comprised of mostly hexagons, with heptagons/octagons at its inner rim and pentagons/tetragons at its outer rim [3]. This is due to the Gaussian curvature distribution of the geometric figure itself. For trivalent graphs, polygons with more than six edges correspond to the loci of negative Gaussian curvature in the 3D embedding of the graph, and vice versa. Ripping off the outer part of the molecule then results in the so-called neck structure, which retains the negatively curved portion only. Now the two ends of the neck are identified with the base edges of two concentric pyramids, which

constitute one-sixth of a double-layer cube as shown in part (b) of the figure. And lastly placing all six identical necks at the right places with their open ends glued together completes the high-genus cube.



Figure 1: Fourfold neck structure and the composition of a genus 5 fullerene. (a) Cutting an appropriate neck structure from a parent toroidal carbon nanotube. The rim of the neck part is drawn in thick line. (b) The neck as sixth of a cubic high-genus fullerene. (c) Completion of the genus 5 molecule.

Making of Beaded High-Genus Sculptures

Following the same strategy provided above one can easily construct beaded models of high-genus fullerenes. First we need to construct the neck structure with beads. The 'unfolded net' is shown in Figure 2(a), where eight-membered rings are threaded with magenta beads and white beads are used in presenting six-membered rings. Note that the beads sit at the middle points of the edges, that is, they represent *chemical bonding* instead of atoms. This is in contrary to traditional commercial molecular model kits where spherical joints serve as atoms and straight sticks connecting the joints represent chemical bonds [4]. For clarity the leftmost beads are repeated at the very right of the figure to satisfy the periodic boundary condition. So in the process of beading, beads marked with empty circles should be identified with the corresponding beads marked with stars. The completed neck is shown in Figure 2(b). Readers familiar with beaded art can easily follow the figures to construct the model. However if this is not the case, readers can refer to [4] for introductory text on beaded fullerenes.



Figure 2: *The construction of beaded neck structure.*

(a) Unfolded Neck structure. The beads marked with empty circles and stars should be identified to close the structure. (b) Simulated beaded neck.

In principle, one can follow exactly the procedure mentioned previous by making all six separated necks and then assemble them into one piece. However, this is not recommended since it would be difficult to thread through the inner layer of the model. Thus the best policy is to have the inner layer of a high-genus sculpture beaded first. The outer part is then 'grown' from these uncompleted necks. Lastly, the whole model is complete by connecting the outer part of the necks.

Other High-Genus Fullerene Embedded on Regular Polyhedra

High-genus fullerenes that approximate four other regular polyhedra can be assembled by neck structures as well, provided that we have chosen appropriate neck structure parameters. For example, fivefold rotational symmetric necks are needed for the construction of regular dodecahedron. Readers of interest are referred to reference [5] for detailed discussions. There is one particular notion worth mention that the three Platonic polyhedra consisting of regular triangles require neck structures different from the situations described above. That is to say, simply changing the rotational symmetry number to three does not result in stable high-genus fullerenes, and the corresponding beaded models are almost impossible to make due to their unreachably high strain. Thus a different type a neck is required which is obtained by ripping off the outer part of another kind of toroidal carbon nanotubes, whose natural rotational symmetry is threefold.



Figure 3:*Photos of High-genus fullerene approximating regular dodecahedron.* (*a*) *Twelve identical fivefold necks joined at their inner parts.* (*b*) *Completed beaded molecule.*

Gallery

Below we present many of our existing collection of beaded high-genus fullerenes. Readers of interest are referred to the blog created by the authors [6].



Figure 4: Photos of beaded high-genus fullerenes. (a) Cube along twofold axis. (b) Fourfold axis. (c)&(d) Truncated tetrahedron.



Figure 4 (continued): *Photos of beaded high-genus fullerenes.* (e)& (f) *Icosidodecahedron.*(g) *Dodecahedron.* (h) *Icosahedron*

Acknowledgements. We wish to thank the National Science Council, Taiwan, R.O.C. for its financial support of this project.

References

[1] B.-Y Jin, C. Chuang, C.-C. Tsoo, *The Wonderful World of Beaded Molecules*, Chemistry (The Chinese Chemical Society, Taipei). Vol. 66, pp. 73-92, 2008, in chinese.

[2] B.-Y. Jin, C. Chuang, C.-C. Tsoo, *Constructing Molecules with Beads: The Geometry of Topologically Nontrivial Fullerenes*, Proceedings of Bridges: Mathematics, Music, Art, Architecture, Culture pp. 391-394, 2010.

[2] C. Chuang, Y.-C. Fan, B.-Y. Jin, *Generalized Classification of Toroidal and Helical Carbon Nanotubes*, J. Chem. Info. Model. Vol. 49, pp. 361-368, 2009.

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

[4] C. Chuang, B.-Y. Jin, Systematics of High-Genus Fullerenes, J. Chem. Info. Model. Vol. 49, pp. 1664-1668, 2009.

[5] <u>http://thebeadedmolecules.blogspot.com</u>.