

Construction of Sierpiński Superfullerenes with the Aid of Zome Geometry: Application to Beaded Molecules

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Abstract

Superfullerenes are a class of complex hypothetical molecules in which each atom of an ordinary fullerene is replaced with yet another fullerene and properly connected to the neighbors accordingly. This self-similarity between the building blocks and the entire structure is known as a Sierpiński sieve. Here we further apply the principle of zome geometry to help construct stable superfullerenes that can serve as models for making beaded molecules. The method has high applicability, and in principle any kind of structure constructed with, for example, Zometool® can be built this way.

Introduction

Since 2010 we have been advertising the idea of constructing physical molecular models using thread and beads. We have been focusing on a large family of molecules called fullerenes, which are composed purely of sp^2 -hybridized carbon atoms. Among its relatives, the buckyball (C_{60}) is the most famous member. Its three discoverers were awarded the Nobel Prize in chemistry in 1996. While these molecules are interesting subjects of chemical research, their structures provide suitable models for constructing beautiful and enduring bead structures.

In particular, at the Bridges 2011 we presented a general scheme for building beaded molecules with high genera, or pictorially having many handles or holes [1]. These high genus fullerenes were assembled from neck-like modules, much like the way of assembling a polyhedron from its constituent polygonal faces. However there is a different way of seeing this divide-and-conquer scheme, inspired by one of the beaded molecules the author made and presented at the JMM art exhibition this year [2]. If we punch holes appropriately in the spherical nodes (C_{60} s) and connect them with straight tubules (carbon nanotubes) according to the polyhedral blueprint, we will have a so-called superfullerene molecule that has the same geometry and topology as the blueprint.

Application of Zome Geometry

The problem now boils down to how to truncate the C_{60} s appropriately to accommodate the connecting carbon nanotubes in a chemically reasonable fashion. While it is crucial to find the precise angles when punching holes in the nodes, there are still considerable difficulties regarding how to do it correctly. This is the place where zome geometry comes to the rescue. Due to the fact that the C_{60} is of icosahedral symmetry, the same as that of the balls of Zometool®, we can first construct a model structure using Zometool. Then, we place C_{60} s (or any other I_h -symmetric Goldberg fullerenes) at the locations of the zome balls in the model structure with identical orientation as the balls. The nice property of zome geometry, or the golden field in terms of abstract algebra, assures that all of the nodes are of the same

spatial orientation. Therefore, it is guaranteed that when connecting the nodes, minimal strain will be present provided suitable carbon nanotubes are chosen for the edges.

There are three basic types of struts in Zometool: yellow, red, and blue. These three different struts correspond respectively to the threefold, fivefold, and twofold rotational axes of the zome ball. To better illustrate the idea, we show here the case of connecting two C_{60} s along one of the twofold axes. As shown in Figure 1, we first build a Zometool model with vZome, the virtual zome model builder authored by Scott Vorthmann. Then the coordinates (trivial in this case, though) are exported on which the C_{60} s are laid. For joining along a twofold axis one needs to truncate two atoms from the C_{60} s each, and a (4,0) carbon nanotube of a certain length is needed for replacing the strut of Zometool and completing the structure.

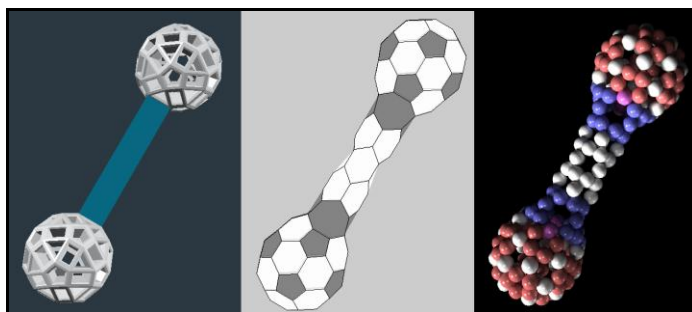


Figure 1: Illustration of replacing zome balls and blue struts with C_{60} s and (4,0) carbon nanotubes. Left: Computer graphics rendered by vZome. Center: The corresponding superfullerene molecule. Right: The corresponding beaded molecule rendered with POV-Ray.

Now the basic idea has been laid out. There are still some realistic limitations for modeling arbitrary zome structures with this technique. For example overlaps of joined parts with struts attached to the ball in close proximity. Apart from that one is able to cover a huge subset of zome structures. We will examine a good part of this subset in this short paper as follows.

Examples of Beaded Superfullerenes with One Type of Strut

Here we show a number of examples each of different geometric features. One can build a cube, regular icosahedron, regular dodecahedron, or truncated icosahedron solely with blue struts of a single length. They are shown in Figure 2. Except for the cube, all of the other three have icosahedral symmetry. While seemingly the cube has an octahedral symmetry, the maximum point group symmetry of the resulting superfullerene is only tetrahedral (T_h), due to the incompatibility of fourfold rotation and the golden field.

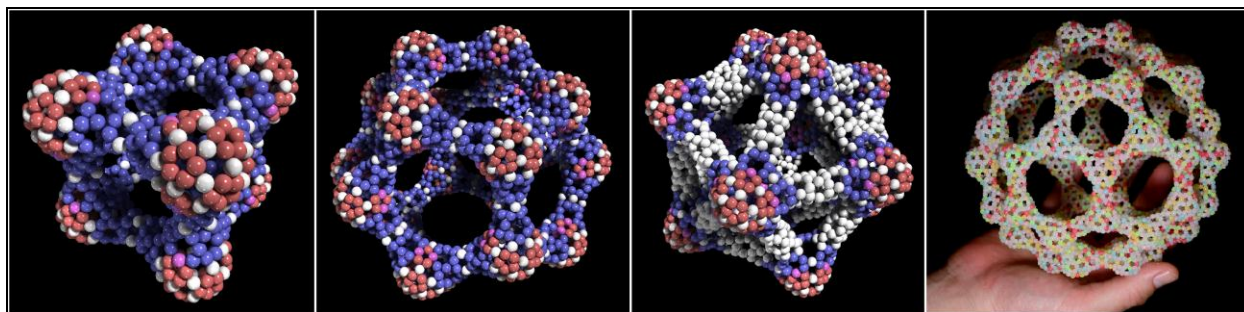


Figure 2: Examples of beaded superfullerene with only one type of (blue) strut. From left to right: Regular cube, dodecahedron, icosahedron, and truncated icosahedron ($C_{60} \otimes C_{60}$). The last one is a real beaded molecule the author (C.C.) managed to make. It will make an appearance in the Art Exhibition.

The truncated icosahedron is worth special attention since C_{60} itself is of the shape of this Archimedean polyhedron. Therefore this structure is of particular interest in the Sierpiński's sense, that there exists similarity between the structure as a whole and its constituent nodes. Along this line, we deliberately adopt the notation of the Kronecker product $A \otimes B$ to denote the result of replacing each node of model structure A by B. Thus, this particular superfullerene is referred to $C_{60} \otimes C_{60}$. Please see our companion paper for more discussion [3]. In fact, Yuan-Jia Fan had designed a Zometool model based on this structure. And one of the authors (BYJ) has led a group of theoretical chemistry students at National Taiwan University to construct it, see Figure 3.

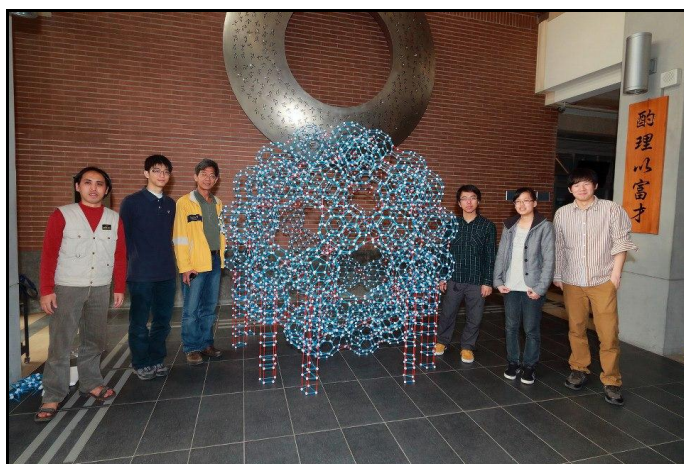


Figure 3: Superfullerene $C_{60} \otimes C_{60}$ built with Zometool. Yuan-Jia Fan and Bih-Yaw Jin are the first and the third on the left, respectively.

Beaded Superfullerenes with More than One Type of Strut

If one incorporates more than one type of Zometool strut, additional complexity arises. The lengths of Zometool struts are determined by the algebraic field to which it belongs. For example the scaling of consecutive levels of the struts is the golden ratio in the golden field. In general it is an approximation to adopt a certain set of carbon nanotube lengths when building such superfullerenes, for there is additional strain energy pertaining to the incommensurability of strut lengths. One therefore has to carefully choose the set of tube lengths for a beaded structure to exist. Here in Figure 4 a trefoil knot and a hypercube are presented. The former is composed of blue struts with three different lengths, and the latter contains blue struts with two different lengths and yellow struts. We note that this method has gone quite beyond the capability of our original approach to constructing high-genus fullerenes [1]. In principle one can build almost any kind of structures of interest as long as they can be simulated with Zometool.

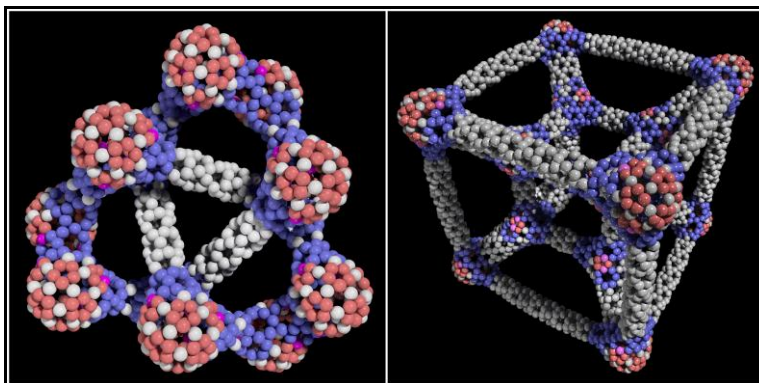


Figure 4: Trefoil knot (left) and hypercube (right) superfullerenes.

Sierpiński Superfullerene: $C_{20} \otimes C_{20} \otimes C_{20}$

The level of the self-similarity described above can be infinite, like that of a Sierpiński triangle. For constructing beaded molecules, there is a strict physical limitation when the size scales up: the structure must hold itself up. This is especially true for Sierpiński superfullerenes since the number of atoms increases steeply as one gets to higher orders of layers. Here in Figure 5 is the simplest nontrivial third level superfullerene implementation: a $C_{20} \otimes C_{20} \otimes C_{20}$ with total 15920 carbon atoms. Although we have not found the time and effort to construct such a gigantic model, it is a beautiful idea by itself that can be seen from simulation already.

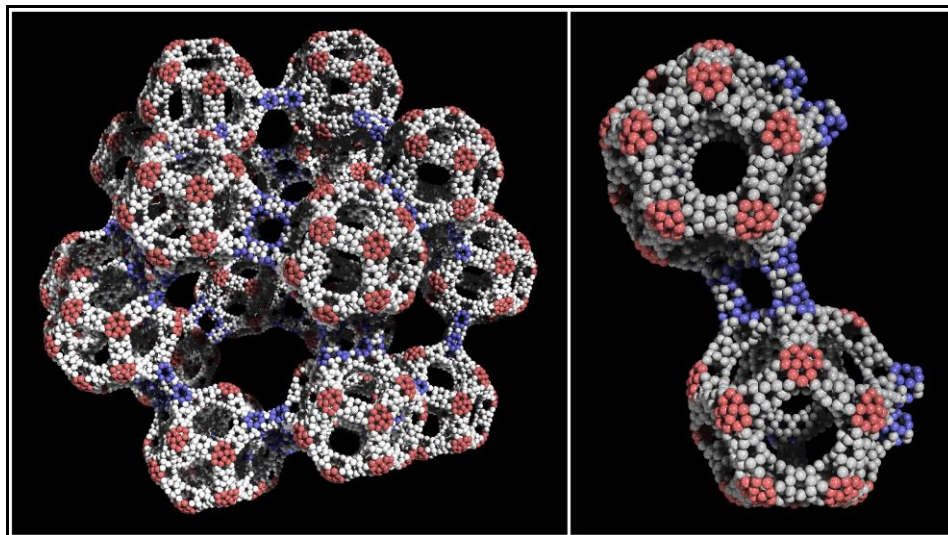


Figure 5: Third order superfullerene: $C_{20} \otimes C_{20} \otimes C_{20}$. We also take out only two adjacent second order nodes for clarity on the right.

Acknowledgements. We wish to thank the National Science Council, Taiwan, R.O.C. for its financial support of this project. We also like to acknowledge the fruitful discussion with Yuan-Jia Fan, and the enthusiastic help from Qian-Rui Huang who wrote the POV-Ray source files used to generate the figures in this paper.

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- [4] For further information please visit our blog: <http://thebeadedmolecules.blogspot.com>.