Designing Skeletal Polyhedral Sculptures Inspired by Octet-Truss Systems and Structural Inorganic Chemistry with Bugle Beads

Chia-Chin Tsoo[a] and Bih-Yaw Jin[b]
[a]National Center for High-Performance Computing, Hsinchu, Taiwan
[b]Department of Chemistry, National Taiwan University, Taipei, Taiwan
E-mail: `c00cct00@nchc.gov.tw`, `byjin@ntu.edu.tw`

Abstract

We employ tubular bugle beads to construct aesthetically pleasing skeletal polyhedral sculptures which may contain nodes with connectivity or coordination number up to twelve. These sculptures can also represent physical models of nanoscale inorganic structures or octet-truss lattice structures. Starting from a few convex deltahedra as fundamental building units, a wide range of skeletal structures inspired by the nanoscale world can be built by using the standard angle weave technique.

Introduction

In the past few Bridges conferences, we have presented a series of studies on the constructing bead models of trivalent graphitic structures and tetravalent extended systems using spherical beads. The trivalent structures include cage-like fullerenes, carbon nanotori, helically coiled carbon nanotubes, high-genus fullerene, carbon Schwarzites, and tetravalent structures comprise all kinds of zeolites and clathrate structures.[1, 2, 3] However, the shape of spherical beads limits their applications mainly to low-connectivity systems and cannot easily be applied to structures with coordination numbers higher than six. Here, in this paper, we will explore the application of bugle beads which are tubular in shape to the construction of skeletal polyhedral structures with coordination numbers up to twelve, which might have potential applications in structural inorganic chemistry and octet-truss systems.

Structural motifs in all of our bugle bead structures consist of the eight convex deltahedra as shown in Fig. 1. The beading technique for making a convex deltahedron is the so-called angle weave which we

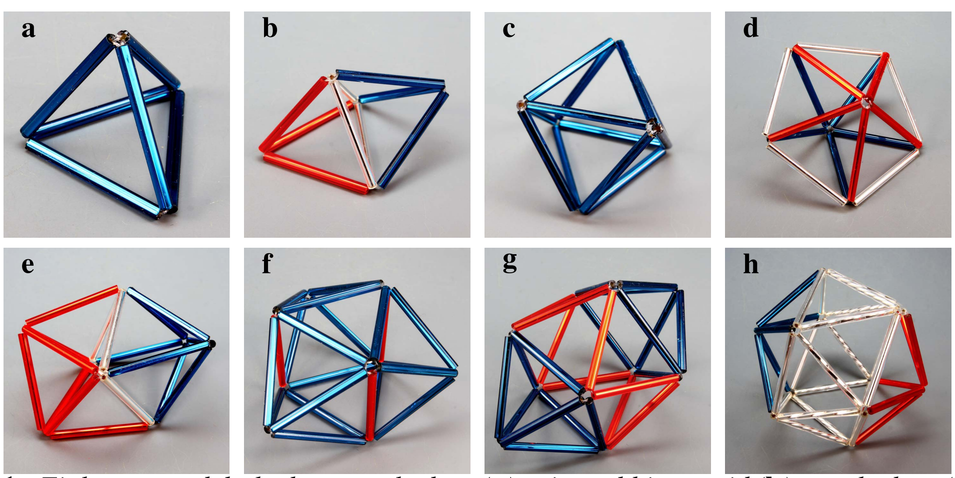

Figure 1 : *Eight convex deltahedra: tetrahedron (**a**), trigonal bipyramid (**b**), octahedron (**c**), pentagonal bipyramid (**d**), snub disphenoid (**e**), tri-augmented triangular prism (**f**), gyro-elongated square bipyramid (**g**), and icosahedron (**h**).*

previously used to make cage-like fullerenes and other periodic trivalent structures. Using the angle weave, every beading step corresponds to creating a triangular face with both ends of fishing line. Note that all bead models discussed in this paper are made by bugle beads with same length equal to 3 cm. The main difference is that faces in all deltahedra are equilateral triangles, and the degrees of vertices can vary from three to five. Therefore, surrounding each vertex, one can have as high as five triangles as in the situation of the icosahedron. If the beading path follows a path that visits each triangular face once and only once, then each bugle bead will be stringed through by the fishing line twice and only twice. The angle defect of each vertex is positive and the whole beaded skeletal structure is rigid as shown by eight beaded deltahedra in Fig. 1. Unlike bead structures based on spherical beads, the stability of a bugle bead structure come from the rigidity of constituent convex deltahedra due to the Cauchy rigidity theorem. Note that these tubular bead structures are in fact hollowed-face or skeletal polyhedra with empty face to see through.

Linked deltahedra

Polyhedral structures appear in nature at different length scales, from the molecular level up to everyday objects. In chemistry, the most useful idealization of molecular structures consists in associating the positions of atoms to the vertices of a polyhedron. Particularly, tetrahedra and octahedra are two most common structural motifs in molecular transition metal chemistry and inorganic solids. Other deltahedra are sometimes important, for instance, the B_{12} groups in the extended structure of B_4C are found to be icosahedra. Many larger structural units in chemistry can be described by linked deltahedra. For instance, two deltahedra can be combined to form a dimer by sharing a common vertex, edge, or face.

In Fig. 2**a**, we show a bead model of two tetrahedra sharing a common vertex. The molecule Cl_2O_7 is an example which has this idealized structure. The second bugle bead model given in Fig 2**b** is the so-called kaleidocycle consisting of a cyclic chain of even number of tetrahedra with two neighboring tetrahedra sharing a common edge. Because the dihedral angle about this common edge is flexible, the whole skeletal kaleidocycle can thus be twisted continually inwards or outwards. The bead model of the Boerdijk-Coxeter helix as shown in Fig. 2**c** shows the third way of combining two tetrahedra by sharing a common face. We deliberately use two different colors for the bead model in Fig. 2**c** so that the tubular beads of the complex that belong to a single tetrahedron form three intertwined helices.

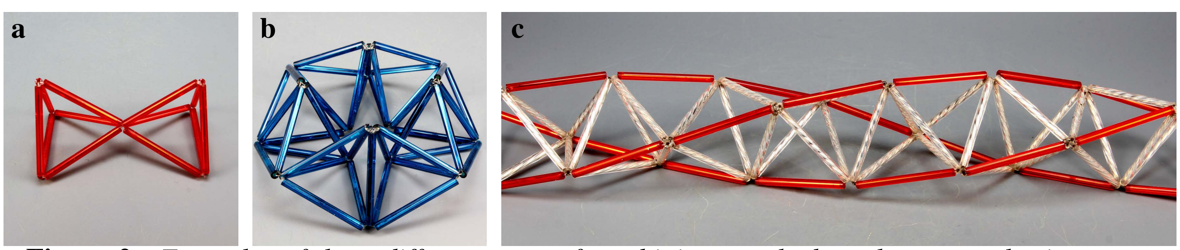

Figure 2: *Examples of three different ways of combining tetrahedra: the vertex-sharing tetrahedral dimer (**a**), the skeletal kaleidocycle consisting of a chain of eight edge-sharing tetrahedra (**b**), and the left-handed form of the Boerdijk-Coxeter tetrahedra (**c**).*

Octet Truss and Icosahedral Systems

In this section, we show that many three-dimensional space frames can be considered as the stacking of these structural motifs. The inherent rigidity of deltahedral building motifs ensures their stability. Physical models given in the first row of Fig. 3 correspond to several octet truss systems based on the stacking of tetrahedra and octahedra. The word "octet" is derived from "octahedron" and "tetrahedron".

The simplest structure of an octet truss is the stella octangula as shown in Fig. 3**a**, which can be created by capping or augmenting each face of an octahedral core by a regular tetrahedron. The result of this face augmentation is a compound formed by two interpenetrated regular tetrahedra with edge length twice of a bugle bead. If one combines octahedra and tetrahedra in a $1 : 2$ ratio, one can get a space filling solid. The most important structure is face center cubic (FCC) lattice as shown in Fig. 3**b**. With slight modification on how close packed sheets are stacked on each other, we get the hexagonal close-packed lattice arrangements (Fig. 3**d**). FCC in the crystal packing is closely related to the octet truss in the space frame. The bead model in Figure 3**c** is a perovskite structure, which is another type of cubic close packed lattice.

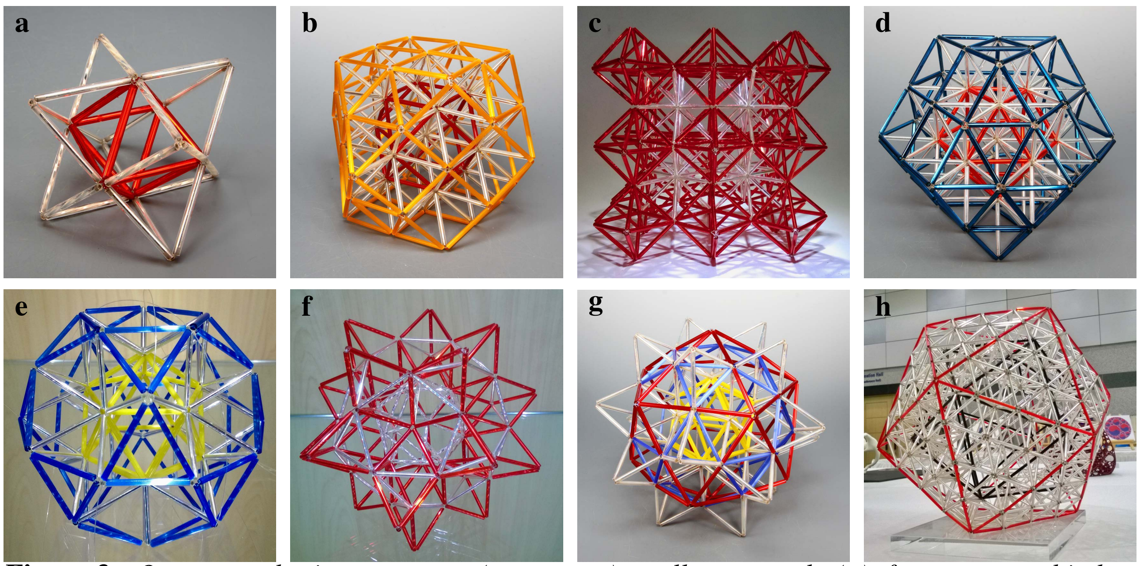

Figure 3: *Octet-truss lattice structures (upper row): stella octangula (**a**), face center cubic lattice (**b**), perovskite (**c**), hexagonal close packing lattice (**d**); Structures with icosahedral symmetry (lower row): icosidodecahedron (**e**) rhombic hexecontahedron (**f**, **g**), frequency-4 Mackay polyhedron (**h**).*

In addition to the octet truss systems, bugle beads can also be used to construct icosahedral skeletal structures as shown in the second row of Fig. 3. The first three sculptures (Figs. 3**e**, **f**, **g**) have similar architectures: they all contain a central icosahedral core, but different kinds of augmentation of deltahedra. The model in Fig. 3**e** has twenty octahedra augmented to the central icosahedron, in such a way that each octahedron share a common face with the central icosahedron and three neighboring octahedra, and the outer skeleton of these octahedra forms an icosidodecahedron. The model in Fig. 3**f** has an extra regular tetrahedron stacked on top of each octahedron. We chose deliberately the red color for certain beads to make the pattern of the rhombic hexecontahedron clear. In Fig. 3**g**, twelve excavated regions along the five-fold axes are augmented by additional twelve pentagonal bipyramids and the resulting structure has an extra frequency-2 Mackay polyhedron. The last model in Fig. 3**h** is also an icosahedral octet-truss structure. Each of its twenty flat faces comprises a single layer of octet truss and twelve excavated tips are augmented by pentagonal bipyramids again to form a two-layer Mackay polyhedron. Inner and outer layers stand for frequency-3 and -4 Mackay polyhedra, respectively.

Polyoxometallates

In this section, we give a final application of bugle beads to polyoxometallates in the structural inorganic chemistry. Polyoxometallates can be considered as a kind of supramolecular architectures resulting from the condensation of coordination polyhedra of transition metal atoms through oxygen bridges. Fig. 4 shows bugle bead models corresponding to the five isomers of Keggin's structures. A classical example of these compounds is ammonium phosphomolybdate which contains the $\mathrm{PMo_{12}O_{40}^{3-}}$ anion discovered in 1826.[4]

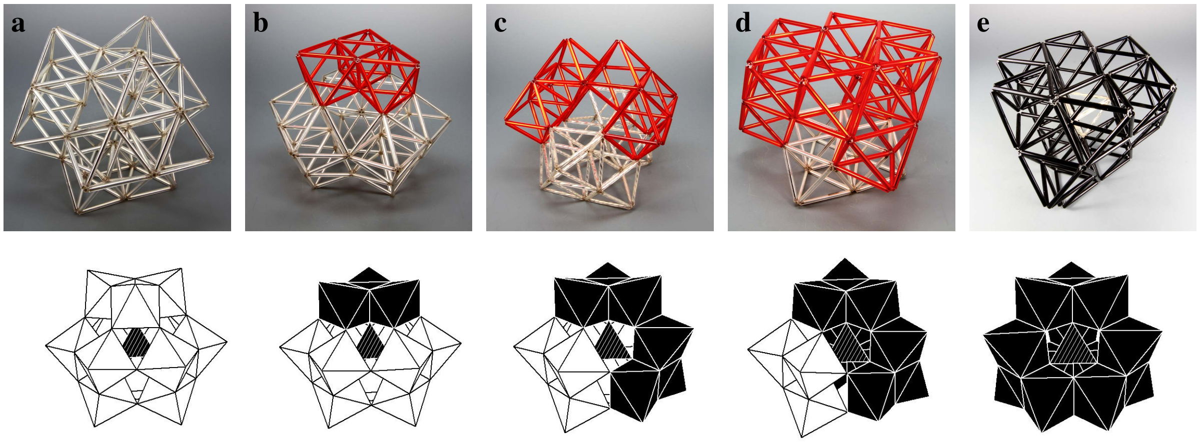

Figure 4 : *Five isomers of Keggin's structure: different isomers are obtained by rotating one or more of the four tri-octahedral units (M_3O_{13}) through* $60°$. *Five schematic plots of Keggin's structures in the second rows are in public domain and were obtained from wikipedia.*

Conclusion

In conclusion, we give a brief description on how tubular beads can be used to construct different kinds of skeletal polyhedral models that can represent physical models of many inorganic structures and octet-truss systems. The nodes in these skeletal structures can have connectivity or coordination numbers up to twelve which is common in many octet-truss lattices. The beading technique we use is the standard right-angle weave that was previously used for trivalent fullerenes and tetravalent periodic zeolite structures. Since we only use bugle beads with the same length in this paper, all deltahedral structures constructed in this paper comprise only four fundamental building motifs. If we use bugle beads with different lengths, a richer structural variety of skeletal polyhedral sculptures can be built.

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