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Architecture of Platonic and Archimedean polyhedral links

QIU WenYuan[1†], ZHAI XinDong[1] & QIU YuanYuan[2]

[1] Department of Chemistry, State Key Laboratory of Applied Organic Chemistry, Lanzhou University, Lanzhou 730000, China;
[2] Faculty of Arts and Social Sciences, The National University of Singapore, SG 117570, Singapore

A new methodology for understanding the construction of polyhedral links has been developed on the basis of the Platonic and Archimedean solids by using our method of the 'three-cross-curve and double-twist-line covering'. There are five classes of polyhedral links that can be explored: the tetrahedral and truncated tetrahedral links; the hexahedral and truncated hexahedral links; the dodecahedral and truncated dodecahedral links; the truncated octahedral and icosahedral links. Our results show that the tetrahedral and truncated tetrahedral links have *T* symmetry; the hexahedral and truncated hexahedral links, as well as the truncated octahedral links, *O* symmetry; the dodecahedral and truncated dodecahedral links, as well as the truncated icosahedral links, *I* symmetry, respectively. This study provides further insight into the molecular design, as well as theoretical characterization, of the DNA and protein catenanes.

knot theory, polyhedron, truncated polyhedron, polyhedral link, DNA catenane, protein catenane

1 Introduction

A fundamental question in chemistry is whether knots and links[1] are new forms of the molecular structures[2,3]. Therefore, the geometrical characteristics and the polyhedral shapes of biological molecules have attracted much attention[4−10], and some of the most exciting discoveries are being made in the controls and syntheses of the polyhedral links or catenanes[11,12], such as the DNA tetrahedron[13,14], DNA cube[15,16], DNA truncated octahedron[17], and the DNA octahedron[18]. A topologically linked protein catenane[19,20], which is a 72-hedral link[8], has been found in the mature empty capsid of the double-stranded DNA bacteriophage. These curious objects have extended our ideas of what is possible in the biochemical world. Many of their most important current questions must be phrased and answered using mathematical methods.

To realize these benefits, an interface between geometry and topology is needed. The challenge that is just now being addressed concerns how to construct a polyhedral link[8] based on Goldberg polyhedra by using the method of the 'three-cross-curve and double-line covering'. Research on Platonic and Archimedean solids is of fundamental importance in understanding the molecular structures. There are only five Platonic solids: the tetrahedron, hexahedron, octahedron, dodecahedron, and icosahedron (http://www.ac-noumea.nc/maths/amc/polyhedr/index.htm). Five of the Archimedean solids, which are derived from the Platonic solids by the process of 'truncation', are well known as the truncated tetrahedron, truncated octahedron, truncated hexahedron, truncated icosahedron, truncated dodecahedron, and so on. It is interesting to note that two or more different polygons appear in each of the Archimedean solids, unlike the Platonic solids which each contain only one single type of polygon (http://www.ul.ie/~cahird/polyhe-

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†Corresponding author (email: wyqiu@lzu.edu.cn)
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dronmode/index.html).

The main goal of this paper is to construct some polyhedral links on the basis of the Platonic and Archimedean solids, as well as its truncated ones. Platonic and Archimedean polyhedral links, the interlinked and interlocked architectures, will reveal interesting new information about molecular structures that have a novel topology. Consideration of the point symmetry group[3,8] has led to the discovery of a new way to detect a polyhedral link whether it is the chirality or just the achirality. Here, we may open the door to understanding and controlling the molecular design and characterization. This progress is the foundation of future development of new models and processes. Using such models, synthetic chemists and biologists are able to test and develop their synthetic strategies.

2 Polyhedral links construction

A polyhedral link[8] can be defined as an interlocked cage constructed from a polyhedron, and the condition for constructing a polyhedral link is that all vertices of the polyhedron are trihedral (of order three). Considering a given polyhedron, if all its vertices are of order three, a corresponding polyhedral link can be directly constructed; otherwise, by the process of truncation, literally cutting off the corners of the polyhedron, a truncated polyhedron and its polyhedral link would be made.

The method for understanding the construction of polyhedral links, in this paper, is called ‘three-cross-curve and double-twist-line covering’ (Figure 1). In general, a polyhedron is a solid of the 3-dimensional space limited by a finite number of faces, vertices, and edges. In particular, a polyhedral link is constructed by using a three-cross-curve (Figure 1(a)) to cover a vertex and using either $2n$ or $2n+1$ double-twist-line ($n=0, 1, 2, \cdots$) to cover an edge (Figure 1(b), (c), and (d)), and then connecting the three-cross-curve with the double-twist-line in polyhedron, respectively. This construction can be utilized to answer some theoretical questions concerning the polyhedral links with $2n$ or $2n+1$ half-twists. Here, $2n$ or $2n+1$ represents the twisting number[3−7], $2n$ is said to be even number of half-twists, and $2n+1$ is said to be odd number of half-twists. Obviously, polyhedral link is an interlocked cage with holes or tunnels, whose boundaries, of course, are the double helix that has the even or odd number of half-twists. More curiously, the three-cross-curve area of the polyhedral link is a novel position of topology which controls molecular shape or size.

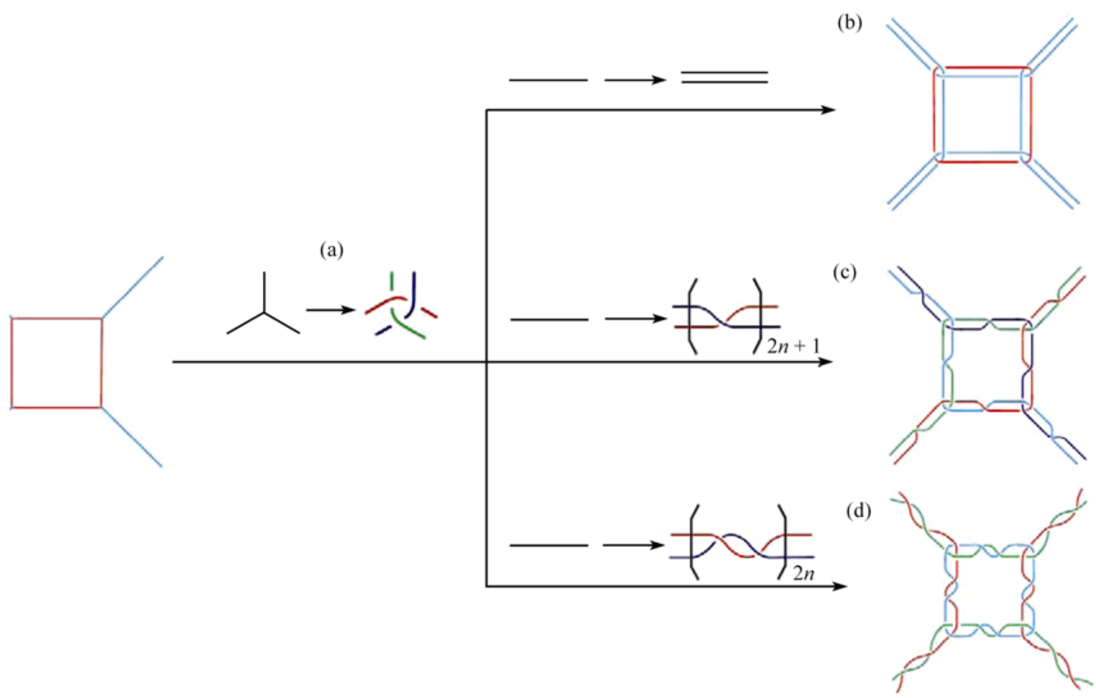

Figure 1 The method for ‘three-cross-curve and double-twist-line covering’.

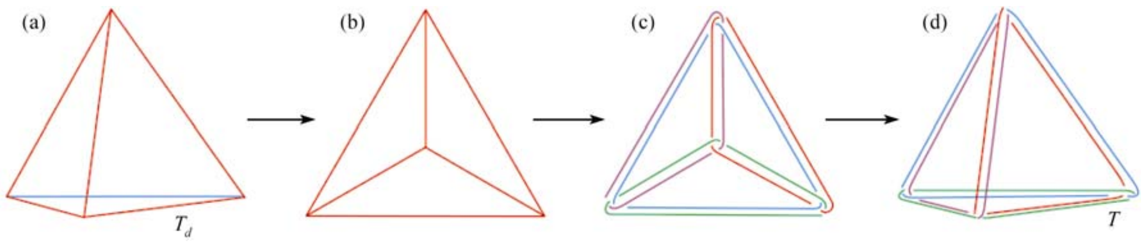

Figure 2 The process of construction for the tetrahedral link with zero half-twist (untwist).

3 Tetrahedral, hexahedral, and dodecahedral links

We know that the tetrahedron, hexahedron, and dodecahedron are featured by trihedral vertices. Thus, some polyhedral links can be directly constructed from these three polyhedra and its truncated polyhedra if all the vertices are trihedral.

For example, the tetrahedron (Figure 2(a)), which has four equilateral triangles, is the simplest of all the polyhedra as it uses the least number of faces to enclose any three-dimensional space. The tetrahedral link is constructed by using 4 three-cross-curve to cover 4 vertices and using 6 double-twist-line to cover 6 edges, and then connecting the three-cross-curve with the double-twist-line, respectively, in the tetrahedron, as shown in Figures 2 and 3.

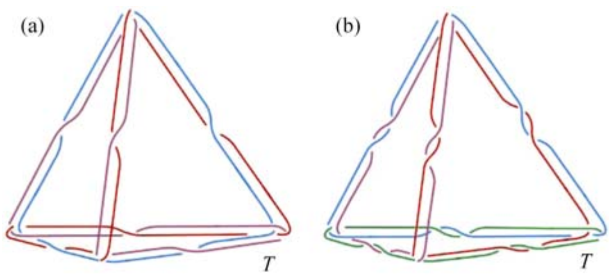

Figure 3 The tetrahedral links with one (a) and two half-twists (b).

If the tetrahedron can be truncated once by symmetrically slicing off each vertex, then the first truncated tetrahedron (8-hedron, Figure 4(a)) is a polyhedron with eight faces, and the first truncated tetrahedral link (8-hedral link, Figure 4(b)) is a nested cage interlocked by four hexagonal rings and four triangular rings.

If the tetrahedron can be truncated twice by symmetrically slicing off each vertex, then the second truncated tetrahedron (20-hedron, Figure 4(c)) is a polyhedron with twenty faces. It is surprising to discover that the second truncated tetrahedral link (20-hedral link, Figure 4(d)) contains four dodecagonal rings, four hexagonal rings, and twelve triangular rings that loop through each other.

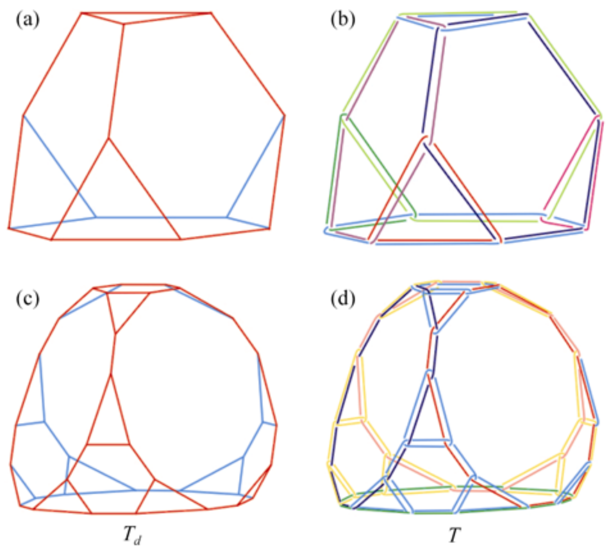

Figure 4 The truncated tetrahedrons ((a) and (c)) and the truncated tetrahedral links ((b) and (d)).

As discussed above, some polyhedral links can also be constructed by using the method of the 'three-cross-curve and double-twist-line covering'. Here are four examples of polyhedral links: the hexahedral and truncated hexahedral links, and the dodecahedral and truncated dodecahedral links, which are, respectively, illustrated in Figures 5—8.

The study of the polyhedral links, from Figure 2 to Figure 8, reveals other outstanding properties:

(1) The symmetrical property of the Platonic polyhedra is one which remains unchanged when it is truncated by symmetrically slicing off each vertex. The tetrahedron and truncated tetrahedrons have T_d group, the hexahedron and truncated hexahedron have O_h group, and the dodecahedron and truncated dodecahedrons have I_h group, respectively.

(2) All symmetry planes in polyhedral links can be vanished without losing esthetic value. The tetrahedral and truncated tetrahedral links have T group, the hexahe-

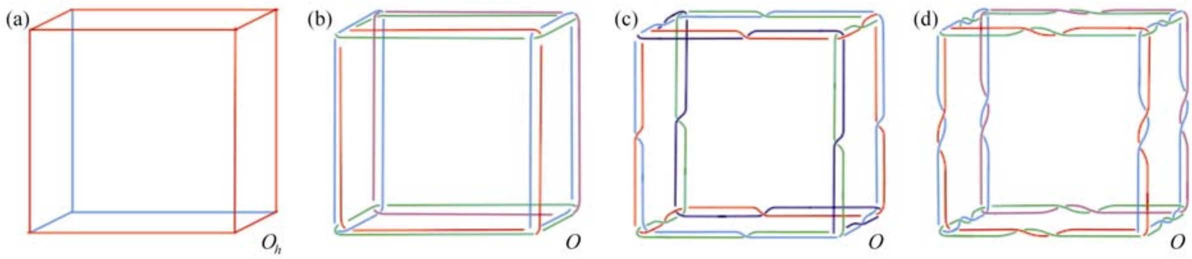

Figure 5 The hexahedron (a) and the hexahedral link with zero (b), one (c), and two half-twists (d).

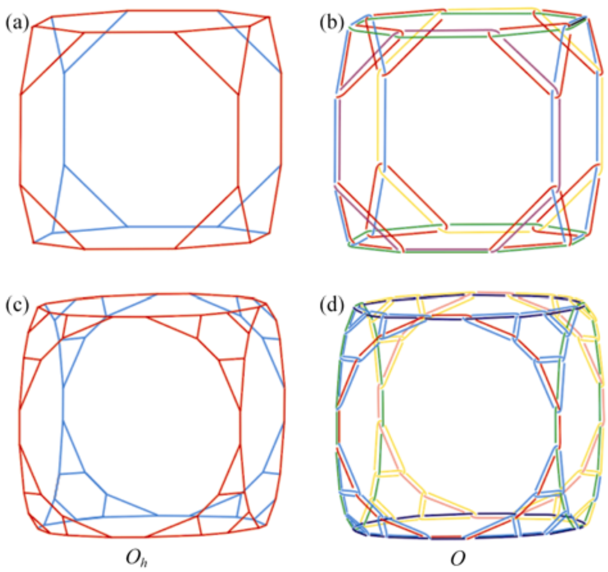

Figure 6 The truncated hexahedrons ((a) and (c)) and the truncated hexahedral links ((b) and (d)).

dral and truncated heaxhedral links have O group, and the dodecahedral links and truncated dodecahedral links have I group, respectively.

(3) The product rules for the tetrahedral, hexahedral, and dodecahedral links, as well as its truncated polyhedral links are respectively written as

$$R_n = 4 + 4\sum_{i=1}^{n} 3^{n-i}\ ;\quad R_n = 6 + 8\sum_{i=1}^{n} 3^{n-i}\ ;$$

$$R_n = 12 + 20\sum_{i=1}^{n} 3^{n-i},$$

where R represents the number of the interlocked rings and n = 1, 2, ⋯.

Today, we can aspire to such goals, in part because of the DNA tetrahedral link[13,14] and the DNA hexahedral link[15,16] which were respectively discovered in the Turberfield's and Seeman's laboratory. These polyhedral links evolved from the interaction between chemistry and biology that appears here in new forms invigorated by new ideas.

4 Truncated octahedral and icosahedral links

We know the octahedron and icosahedron, whose vertices are respectively of order 4 and 5 (Figure 9). Unfortunately, the octahedral and icosahedral links cannot be obtained using our method. If we can make two truncated polyhedra, by cutting all 'corners' of these two polyhedra, whose vertices are all of order 3, then the truncated octahedral and icosahedral links can only be constructed.

In order to describe our ideas, for instance, two results of the truncated octahedrons are shown in Figure 10: the first truncated octahedron (14-hedron, Figure 10(a)) contains six square faces and eight hexagonal faces; the second truncated octahedron (38-hedron, Figure 10(c)) contains six octagonal faces, eight dodecagonal faces, and twenty-four triangles.

The truncated octahedral links can be constructed on

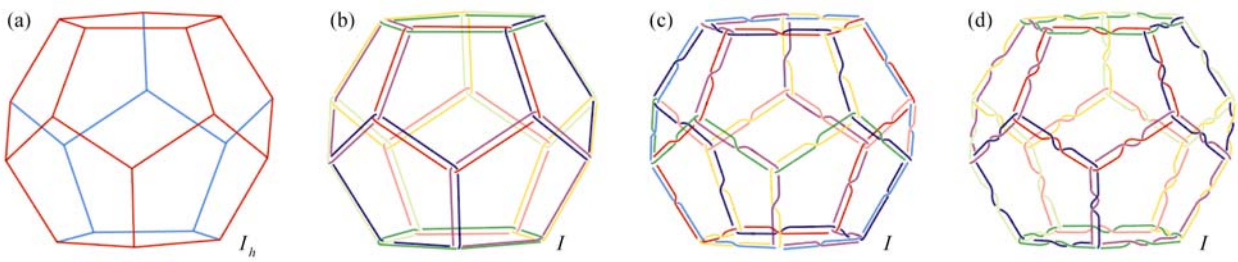

Figure 7 The dodecahedron (a) and the dodecahedral links with zero (b), one (c), and two half-twists (d).

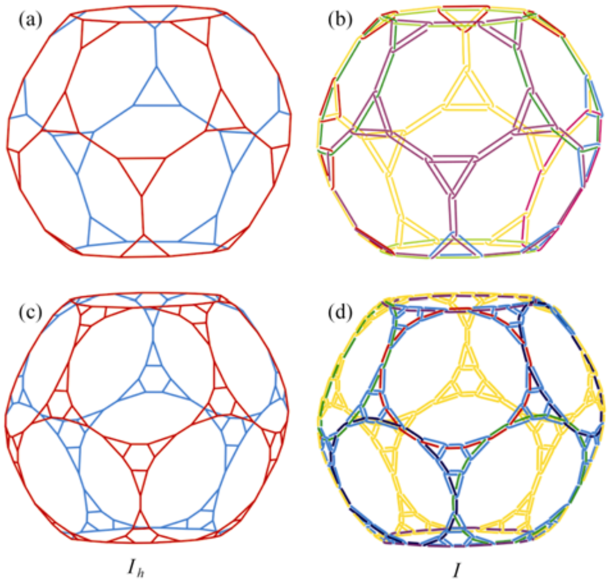

Figure 8 The truncated dodecahedrons ((a) and (c)) and the truncated dodecahedral links ((b) and (d)).

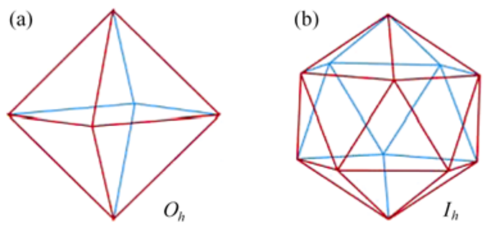

Figure 9 The octahedron (a) and the icosahedron (b).

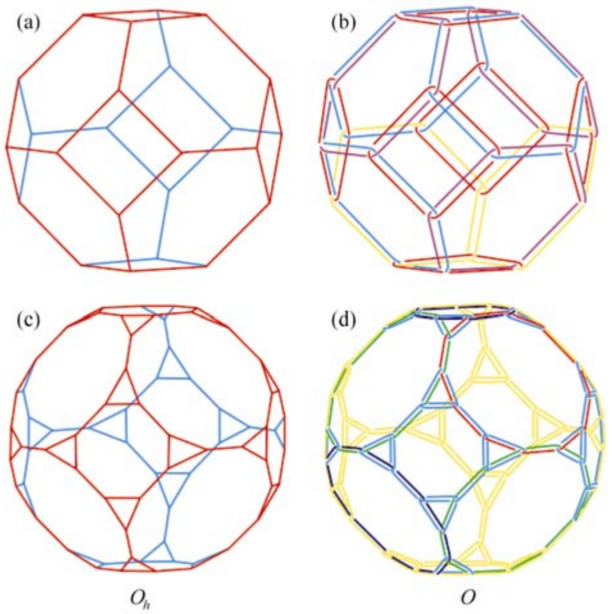

Figure 10 The truncated octahedrons ((a) and (c)) and truncated octahedral links ((b) and (d)).

the basis of the truncated octahedrons: the first truncated octahedral link (14-hedral link, Figure 10(b)) is a nested cage interlocked by 8 hexagonal rings and 6 quadrangular rings; the second truncated octahedral link (38-hedral link, Figure 10(d)) is composed of 8 dodecagonal rings, 6 octagonal rings, and 24 triangular rings that loop through each other.

To discover the others, we have to tire ourselves a little and proceed with the following method: by cutting the 'peaks' of an icosahedron (Figure 9(b)), we obtain the first truncated icosahedron (32-hedron, Figure 11(a)) whose faces are the faces of 12 regular pentagons and 20 hexagons. Applying such a truncation to Figure 11(a) leads to the second truncated icosahedron (92-hedron, Figure 11(c)) whose faces are the faces of 20 dodecagons, 12 decagons, and 60 triangles.

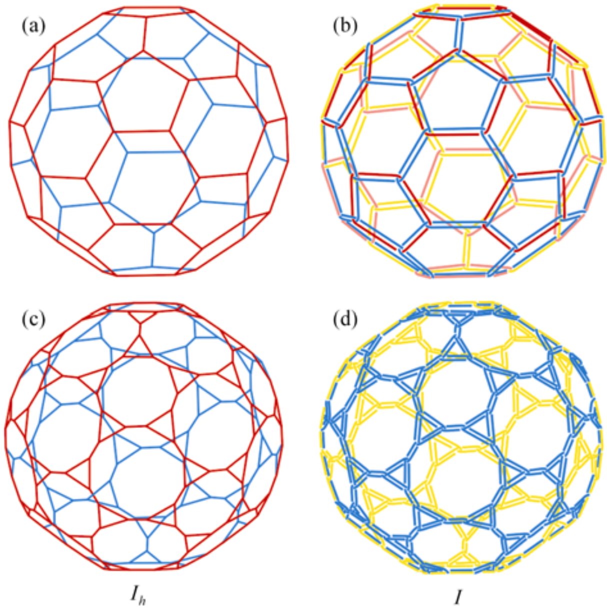

Figure 11 The truncated icosahedrons ((a) and (c)) and truncated icosahedral links ((b) and (d)).

The truncated icosahedral links can also be constructed by using the above method. It should be noted that the first truncated icosahedral link (32-hedral link, Figure 11(b)) is an interlocked cage interlinked by 12 pentagonal rings and 20 hexagonal rings, and the second truncated icosahedral link (92-hedral link, Figure 11(d)) consists of 20 dodecagonal rings, 12 decagonal rings, and 60 triangular rings that loop through each other.

Observing both of the polyhedra and the polyhedral links above, it can be clearly seen that the octahedron and truncated octahedrons have O_h symmetry group, and the truncated octahedral links have O symmetry group; the icosahedron and the truncated icosahedrons have I_h symmetry group, while the truncated icosahedral links have I symmetry group. Unlike polyhedra, the polyhedral links have no plane of symmetry.

It is also worth noting that the product rules for the truncated octahedral and icosahedral links are respectively written as

$$R_n = 8 + 6\left[1 + 4\sum_{i=2}^{n} 3^{n-i}\right]; \quad R_n = 20 + 12\left[1 + 5\sum_{i=2}^{n} 3^{n-i}\right],$$

where R represents the number of the interlocked rings and $n = 2, 3, \cdots$.

The experimental development of the new techniques to construct these polyhedral links has been paid off handsomely. The degree to which these polyhedral links of control achieved is shown in the synthesis of DNA truncated octahedral link[17] and the characterization of HK97 bacteriophage capsids[19,20]. At another extreme example like DNA octahedral link[18], with each edge made of two interlinked DNA double helices, it is judged to be hopefully targeted for the novel structures of the polyhedral links.

5 Results and discussion

This study has presented a new approach to construct polyhedral links based on the Platonic and Archimedean polyhedra, which provides new ideas for the molecular design and theoretical characterization of the DNA and protein catenanes. The tetrahedral links, hexahedral links, and dodecahedral links can be respectively constructed from the tetrahedron, hexahedron, and dodecahedron. However, since the vertices of the other two Platonic solids, the octahedron and icosahedron, are of order 4 and 5, respectively; the corresponding polyhedral links can only be constructed by the process of truncation.

Our results show that the tetrahedral and truncated tetrahedral links have T symmetry; the hexahedral and truncated hexahedral links, as well as the truncated octahedral links, O symmetry; the dodecahedral and truncated dodecahedral links, as well as the truncated icosahedral links, I symmetry, respectively. In particular, there are no planes of symmetry in the groups T, O, and I, thus all these polyhedral links are chiral and the right-handed and left-handed forms are distinct. In other words, polyhedral links have a property of the topological rubber glove[3], because it can be turned inside-out, but the inside and outside are not the same, i.e., if a right-handed polyhedral link is turned inside-out, it is converted into a left-handed polyhedral link.

Most importantly, these polyhedral links have some holes that are small, and the others are large. There is a great possibility that the small holes are the molecular skeletons, whereas the large holes are a network of tunnels as if some 'creatures' travel through them. Although there is much to probe, the idea is simple but brilliant, as many important scientific research ideas are.

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