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Extended Goldberg polyhedral links with even tangles

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Abstract

A new methodology for understanding the construction of polyhedral links has been developed on the basis of 4-regular polyhedra and knot theory. In the method, we utilize uniform $2n$-tangles (n is an integer) to cover all vertexes of Extended Goldberg polyhedra, and many infinite series of interlinked and interlocked architectures have been assembled. The growth rule of links with tangle of $|n| = 1$ and a class of topological transformation depending on the number of n are systematic enumerated. Our study reveals that these novel structures all have I symmetry and each belongs to a given topological configuration, D or L. Moreover, they provide some potential models for protein and DNA cages which have chirality.

1. Introduction

Polyhedral links, or chemically known as polyhedral catenanes, an uncommon feature of molecular architectures, have been the extraordinary topological objects of interest and study in recent decades [1-5]. Organic catenanes, which are formed by macrocycles, and DNA catenanes looped through circular single strand of DNA, have been synthesized in the laboratory [6-17]. At the same time, the theoretical treatment and description of these non-trivial molecular structures were developed in the field of knot theory [18-22], which study and quantization of configurations of simple closed curves in Euclidean 3-space. Taking inspiration from molecular entanglement in biology, as seen in the topologically linked 72-hedral protein rings of capsid [23], Qiu et al [24, 25] constructed some beautiful links based on Goldberg polyhedra and carbon nanotubes. Now, the underling topological principle of chemical catenanes brings new challenges and opportunities for making connections between mathematics and chemistry.

From biology to chemistry, polyhedra are the well known high-symmetry fashions to mimic many substances in nature [26, 27]. Hence, their regular property allows them to serve as possible candidate backbones for chemical catenanes. Here, we focus on two series of novel geometrical objects with icosahedral symmetry [28-31]. Rotate-Extended polyhedra, defined as Γ (3, 0) –Goldberg polyhedra, and Stretch-Extended Goldberg, defined as Γ (3, 4) –Goldberg polyhedra. Their numbers of vertices and edges, respectively, satisfy the following equations:

$$V_R = 30(h^2 + hk + k^2)\ ;\quad V_S = 60(h^2 + hk + k^2)\ ;$$

$$F_R = 30(h^2 + hk + k^2) + 2\ ;\quad F_S = 60(h^2 + hk + k^2) + 2\ .$$

Where h and k are two integers and $0 < h \geq k \geq 0$ and have been defined as a two dimensional Goldberg vector G = (h, k) [32]. In particular, these 4-regular polyhedra, i.e. four edges meet at each vertex, can be used to describe the surfaces of icosahedral capsids [33, 34] which are not covered by Goldberg polyhedra.

This article combines tangle theory [1] with Extended Goldberg polyhedra, and proposes a new approach for description of polyhedral links with *I* symmetry. Tangles, the fundamental unit of knotted and catenated topologies, can be divided into odd and even types depending on their half-twist numbers. We find that structures obtained by even tangles can find their application in molding biomolecules, thus, this paper will consider only even tangles. Research on the chiral criterion and topological transformation of these polyhedral links may aids in understanding the molecular design and assembly principle of protein catenanes, and offers a new route to DNA polyhedral catenanes. Moreover, these chiral polyhedral links may provide some theoretical models for icosahedral viral capsids [35], which possess handedness.

For convenience, we denote Goldberg polyhedra and their links by *GP* and *GPL*, Rotate-Extended Goldberg polyhedra and their links by *REGP* and *REGPL*, Stretch-Extended Goldberg polyhedra and their links by *SEGP* and *SEGPL*.

2. Fabrication

Definition 1. In knot or link diagrams *D*, a tangle *A* is a region in the projection plane with four emerging arcs surrounded by a circle. Furthermore, there are four points where the knot or link crosses the circle as occurring in the four fixed directions {*NW*, *NE*, *SW*, *SE*}. We define that *A* as a positive tangle when it is resulted by left-handed twists, and it is considered to be negative when it has only right-handed twists.

It appears that the tangle embedding theory has been applied to model DNA recombination and protein-DNA binding successfully [36-38]. From the point of view of molecular design, tangles can also be used as the building blocks of knot and link projections, thus, the identical unit tangles can be assembled into predesigned topologies. In our approach of which defined as *tangle composition*, the construction of polyhedral links will satisfy the following three processes:

(i) Tangles selection. Using even (*2n*) tangles as the fundamental unit to replace all the four-valent vertices of *EGP*, and the absolute value $|n|$ denotes that the number of half-twists which are put in a tangle. Thus, there are some full-turn twists contained in an even tangle, and the overpass crossing and underpass crossings appear in pair wise. Figure 1 illustrates four different tangles with n of ±1 and ±2. In general, there are two crossings emerging when $n = \pm 1$ and four crossings emerging when $n = \pm 2$.

(ii) Tangles position. We define the external space S^e are the regions between the end of the *NW* and *SW* or *NE* and *SE*. When fixing the tangles on vertices, the four arcs will superpose the four edges coming out from the same vertex, then ensure S^e will distribute on the 3-gonal faces of a *REGP* or 4-gonal faces of a *SEGP*.

(iii) Tangles connection. Connecting the arc end of a tangle to the arc end of four adjoining tangles along edges, then some alternating *EGPLs* and *SGPLs* with even tangles at their vertices are obtained.

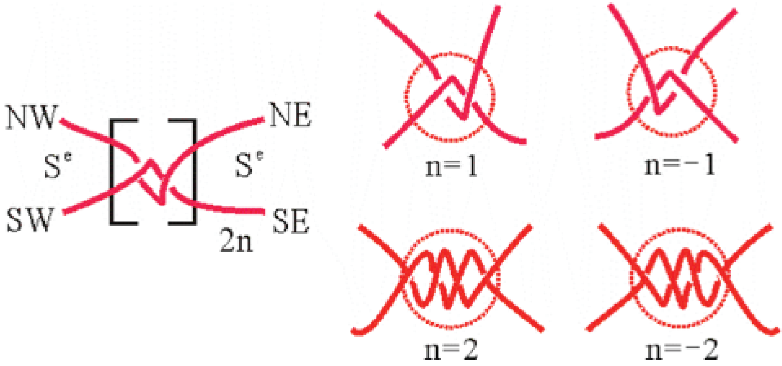

Figure 1. Even tangles obtained by 2*n* half-twists

As a result, 5-member and 6-member rings will be occurred in *EGPL*, and 5-member, 6-member and 3-member rings are interwound with even number of crossings in *SGPL.* Thus, for two infinite series polyhedral links, the number of components C_R and C_S, and the number of crossings N_R and N_S can be easy calculated by following equations:

$$C_R = R_5 + R_6 = 10(h^2 + hk + k^2) + 2\,;\; C_S = R_5 + R_6 + R_3 = 30(h^2 + hk + k^2) + 2\,;$$

$$N_R = 2nV = 60n(h^2 + hk + k^2)\,;\;\; N_S = 2nV = 120n(h^2 + hk + k^2).$$

In addition, the pattern of twists in tangles of polyhedral links destroys the reflection operations of icosahedral symmetry, and then these links only retain the rotational symmetry of icosahedrons. It means that they are belonged to the point group *I*, therefore, chiral.

Definition 2. Given an oriented link *K,* the linking number *L* (*K*) is one half the sums of the characteristics (i.e., the crossing number +1 or -1 which was notated by reference [1]) of the intercomponent crossings. It has been defined that the link as *D* configuration if *L* (*K*) > 0, whereas the link is *L* configuration if *L* (*K*) < 0 [39].

The linking number is an invariant of *K*, thus, *L* (*K*) can be used to help us to determine the chirality of the orientated link. According to our design, if all rings are given the same orientation, the linking number of a *GPL* corresponds to the number of full turn twists at all vertexes. By definition 1 and 2, we can conclude that the positive tangles yield *D* polyhedral links, whose linking numbers are positive, if, conversely, the negative tangles will yield *L* polyhedral links, whose linking numbers are negative. These two different configurations cannot be interconvert by continuous deformation. Thus, they exit as a pair of topological enantiomorphs.

3. The links with 2 and -2 tangle

In this section, the results of links with 2 and -2 tangle ($|n| = 1$) is systematic enumerated in "racemic" pairs. In addition, graphic illustrations of these topological structures are presented into two classes depending on the symmetry of original polyhedra. In particular, these polyhedral links may provide some potential models for icosahedral viral capsids which possess chirality. Such as the handedness of herpes simplex virus capsid is not caused by its nonskew surface lattice, and it may be generated from the entanglement of side-chain amino acid each other by covalently bond to hook the asymmetric triplexes, which provide a particular stabilization mechanism [35]. Furthermore, each viral capsid favors a unique chirality due to the properties of spontaneous broken symmetry, which are of considerable biological interest. Thus, capsids with levo and dextro form may be characterized by *L* and *D* polyhedral links, respectively.

3.1. The first type polyhedral links

The symmetry of *EGP* depends on Goldberg vector $G = (h, k)$ [32]. When G = (h, 0) or (h, h), the corresponding series of achiral *EGP* have the full I_h point group, then the type I *EGPL* with only rotational point group *I* are generated by our method above. Therefore, the mirror plane of polyhedra is disappeared in this process and the chirality is caused. The first three members of this type *EGPL* are depicted in the following parts.

The first case, if

$$G = (1,0), F = 30(h^2 + hk + k^2) + 2 = 30(1^2 + 1\times 0 + 0^2) + 2 = 32$$

and

$$F = 60(h^2 + hk + k^2) + 2 = 60(1^2 + 1\times 0 + 0^2) + 2 = 62,$$

then the I (3,0)-32 and the I (3,4)-62-polyhedral links are obtained (Figure 2, 3). They all exist as topological enantiomorphs, of $n = 1$, the corresponding configuration is D, whereas of $n = -1$, the corresponding configuration is L. For the I (3, 0)-32 - polyhedral link, the number of components and crossings are

$$C_R = 10(1^2 + 1\times 0 + 0^2) + 2 = 12\,,\quad N_R = 60(1^2 + 1\times 0 + 0^2) = 60\,.$$

For the I（3,4）-62 - polyhedral link, the number of components and crossings are

$$C_S = 30(1^2 + 1\times 0 + 0^2) + 2 = 32\,,\quad N_S = 120(1^2 + 1\times 0 + 0^2) = 120\,.$$

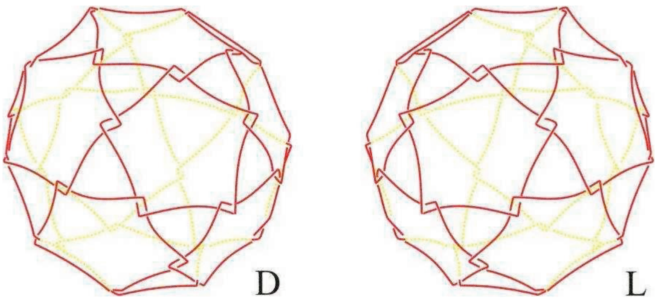

Figure 2. I (3, 0)-32-hedral links. The D configuration link derived from a polyhedron by using 2 tangles to cover vertexes; the L configuration link derived from a polyhedron by using -2 tangles to cover vertexes. The orientations of all rings are same.

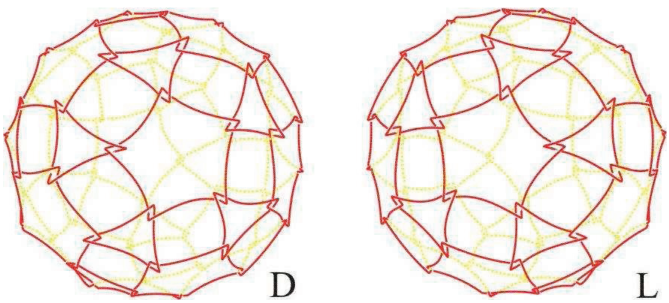

Figure 3. I (3, 4)-62-hedral links with |2| tangles of D and L configuration

If

$$G = (1,1), F = 30(1^2 + 1\times1 + 1^2) + 2 = 92$$

and

$$F = 60(1^2 + 1\times1 + 1^2) + 2 = 182\ ,$$

then the *I* (3, 0)-92 and the *I* (3, 4)-182-polyhedral links are obtained (Figure 4, 5). For the *I* (3, 0)-92-polyhedral link, the crossing number N_R is 180, the component number C_R is 32, which includes 12 pentagonal rings and 20 hexangular rings. By rings, we mean an unknotted closed polygonal curve. For the *I* (3, 4)-182-polyhedral link, the crossing number N_R is 180, the component number C_R is 32, which include 12 pentagonal, 20 hexangular and 60 triangular rings.

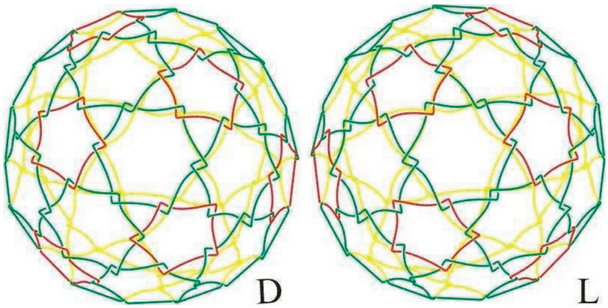

Figure 4. *I* (3, 0)-92-hedral links with |2| tangles of *D* and *L* configuration

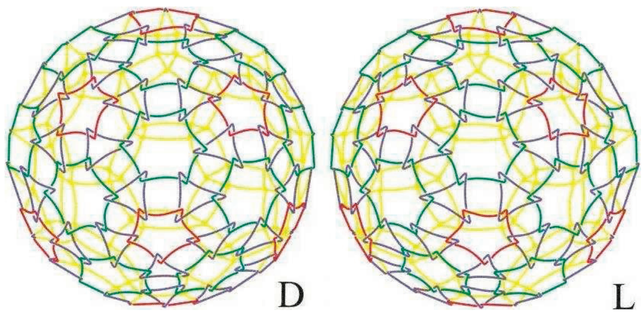

Figure 5. *I* (3, 4)-182-hedral links with |2| tangles of *D* and *L* configuration

If

$$G = (2,0), F = 30(2^2 + 2\times 0 + 0^2) + 2 = 122$$

and

$$F = 60(1^2 + 1\times 1 + 1^2) + 2 = 242\,,$$

then the *I* (3, 0)-122 and the *I* (3, 4)-242-polyhedral links are obtained (Figure 6, 7). For the *I* (3, 0)-122-polyhedral link, the crossing number N_R is 240, the component number C_R is 42, which include 12 pentagonal rings and 30 hexangular rings. For the *I* (3, 4)-242-polyhedral link, the crossing number N_R is 480, the component number C_R is 122, which includes 12 pentagonal, 30 hexangular and 180 triangular rings.

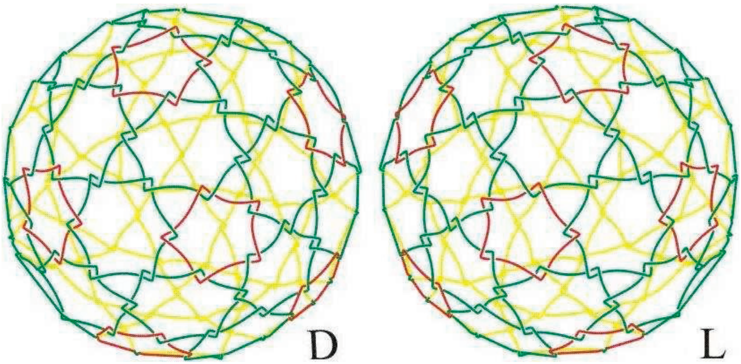

Figure 6. *I* (3, 0)-122-hedral links with |2| tangles of *D* and *L* configuration

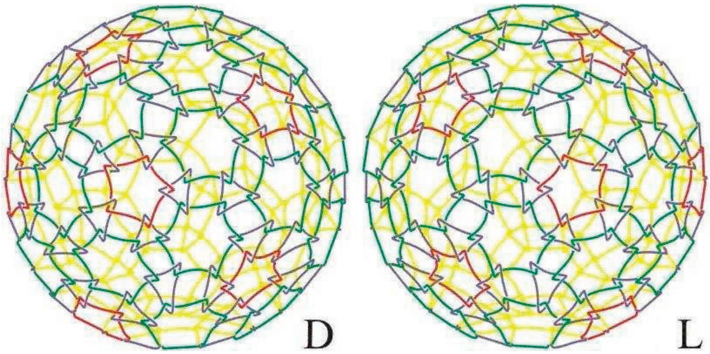

Figure 7. *I* (3, 4)-242-hedral links with |2| tangles of *D* and *L* configuration

3.2. The second type polyhedral links

In contrast with the type I *EGPL*, the series of type II polyhedral links are obtained from *EGP* with *I* symmetry, which is related to Goldberg vector G (*h*, *k*), where 0 < h < k. Hence, the symmetry remains unchanged and the chirality is maintained in this process. The following are some examples of the type II *EGPL*.

If

$$G = (2,1), F = 30(h^2 + hk + k^2) + 2 = 30(2^2 + 2\times 1 + 1^2) + 2 = 212$$

and

$$F = 60(h^2 + hk + k^2) + 2 = 60(2^2 + 2\times 1 + 2^2) + 2 = 422\,,$$

the *I* (3, 0)-212 and *I* (3, 4)-422-polyhedral links are obtained (Figure 8, 9). For the *I* (3, 0)-212-polyhedral link, its component number C_R = 10(2^2+2×1+1^2)+2 = 72, and its crossing number N_R = 60(2^2+2×1+1^2) = 420. For the *I* (3, 4)-422-polyhedral link, its component number C_S = 120(2^2+2×1+1^2)+2 = 212, and its crossing number N_S = 120(2^2+2×1+1^2) = 840.

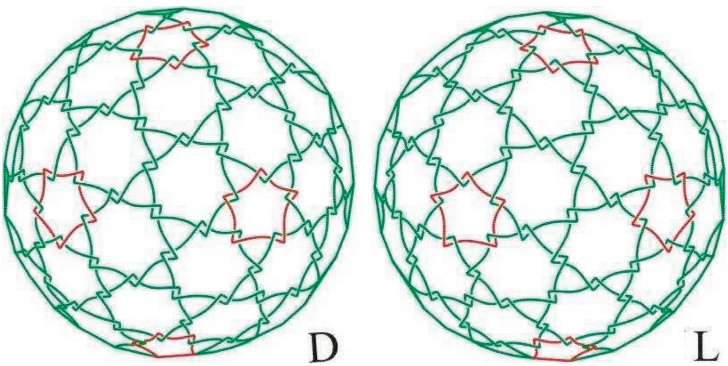

Figure 8. *I* (3, 0)-212-hedral links with |2| tangles of *D* and *L* configuration

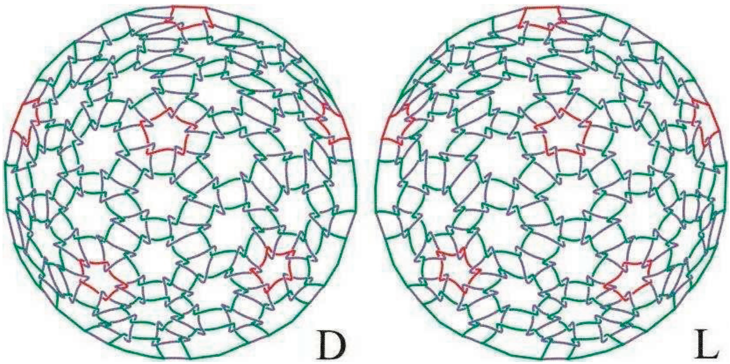

Figure 9. *I* (3, 4)-422-hedral links with |2| tangles of *D* and *L* configuration

If G = (3, 1), F = $30(3^2+3\times1+1^2)+2 = 392$ and F = $60(3^2+3\times1+1^2)+2 = 782$, then the *I* (3,0)-392 and *I* (3,4)-782-polyhedral links are obtained (Figure 10, 11). For the *I* (3, 0)-392-polyhedral link, the crossing number $N_R = 780$, the component number $C_R = 132$, which are nested cages interlocked by 12 pentagonal rings and hexangular rings. For the *I* (3, 4)-782-polyhedral link, the crossing number $N_S = 1560$, the component number $C_S = 392$, which are nested cages interlocked by 12 pentagonal, 120 hexangular and 260 triangular rings.

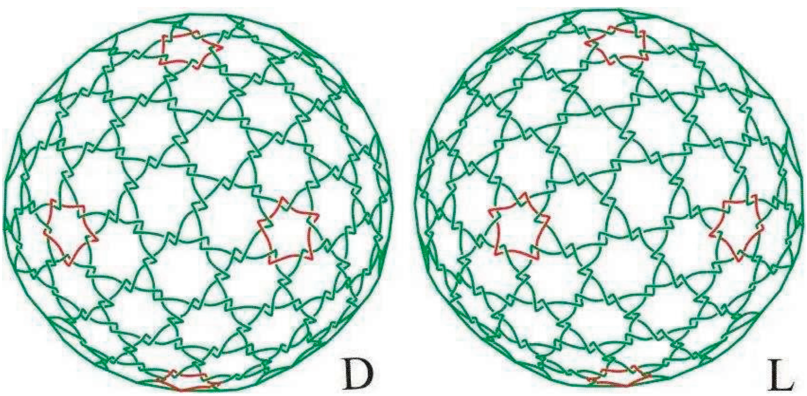

Figure 10. *I* (3, 0)-392-hedral links with |2| tangles of *D* and *L* configuration

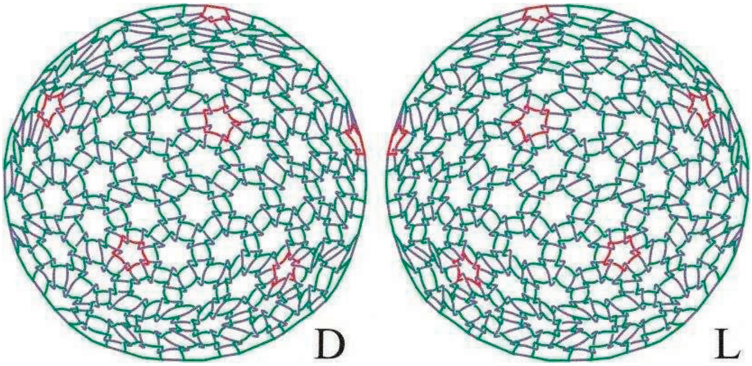

Figure 11. *I* (3, 4)-782-hedral links with |2| tangles of *D* and *L* configuration

4. The topological transformation of links

Symmetry plays an important role as the guiding principle for the design of novel molecules, thus, the point symmetry group *I* herein is an invariant characteristic and criteria for topological chirality of a polyhedral link. It is shown that if we retain the rigidly presentation with *I* symmetry, such a transformation as alter the number of tangle *2n* leads to many other infinite series of links whose members are different isotopy types. Such as $n = \pm 2$, whose link graphs is illustrated in Figure 12, by using tangles with two full twists to cover vertexes of polyhedra, and the obtained structures are not topological equivalent to the links with one full twist when $n = \pm 1$. As a conclusion, the topological transformation has the following distinctive features:

(i) The *2n* tangle at each vertex positively adds a same configurationally full twist at a time, such the configuration of vertexes will transfers to every edges step by step and form double-helix structures finally. This change means that nicks one strand of the tangle open, twists it once around the other strand, and reglues the two ends together. Assuming the axis still lies in a plane, we have increased or decreased each of *L* (*K*) by one operation.

This mathematical phenomenon also has interesting implications for biochemistry, and nature gets around this problem by providing enzymes called topoisomerases. Suppose now that an enzyme add or remove 10.5 base pairs per twist after one DNA recombination. If considering of tangled DNA as a ribbon, then the central line of the ribbon is referred to as the helix axis of the DNA molecule-the polyhedral backbone. It has been proved that the linking number $L(K)$ can be split into two geometric properties called the average writhe Wr and the twist Tw, which is expressed by the White equation $L(K) = Wr + Tw$ [22]. In our final models, the linking number $L(K)$ is equal to the twist Tw, then $Wr = 0$. Thus, a polyhedral link is not the supercoiling of the DNA strands and the helix axis (polyhedral backbones) can been transformed into a plane graph.

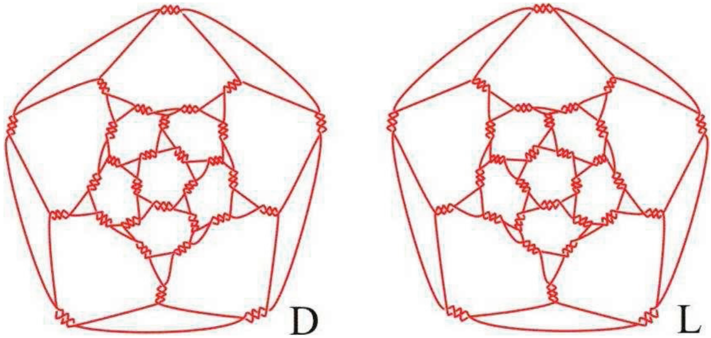

Figure 12. The plane graphs of *I* (3, 0)-32-hedral links with |4| tangles

(ii) The external space S^e will be gradually shrinking, in general, S^e which distribute on the 3-gonal faces shrink into vertex conformation of three branches, and S^e which distribute on the 4-gonal faces collapse into vertex conformation of four branches. Finally, if n is large enough, the backbone structures of polyhedral links will undergo deformations, which named "triangle -collapsing" and "quadrangle- collapsing", i.e. the inverse of truncation of 3-regular and 4-regular vertices. In general, a *REGPL* will be transformed into a new form of *GPL*, and a *SEGRL* will be transformed into a new form of *REGPL*. Two examples of these new nested structures, which are illustrated in Figure 13, are obtained by the topological transformation from *I* (3, 0)-32 and *I* (3, 4)-62- polyhedral links. During the process, all the polyhedral links preserve their absolute configuration, in these two cases, *D*.

It is interesting to note that adding the different base-pair sequences to these pure mathematical structures, the resulting constructions are similar to DNA catenanes. Recently, some large 3-dimension structures such as dodecahedra (12-hedron) and buckyball

(32-hedron) have been designed to self-assembly by DNA [17]. Further considering this topological transformation with the augmentation of twist number *n*, we see that the polyhedral backbone of links will undergo a geometric deformation in agreement with the topological requirement, then spring into some infinite series of new polyhedral links. It means that this non-isotopic transformation may guide the experiment and suggested as a possible synthetic route, which is topology-support-geometry, i.e. the geometric backbone of polyhedral links is decided by the predetermined topological structure of polyhedral links.

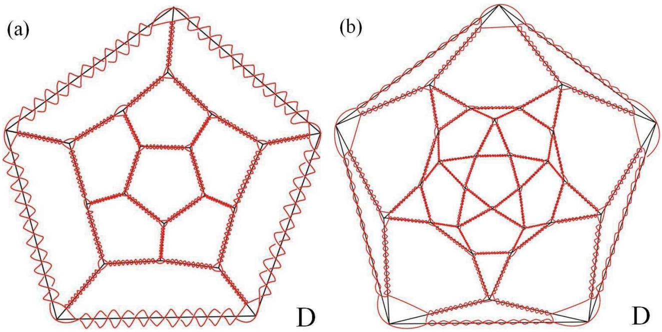

Figure 13. (a) The 12-polyhedral links derived from *I* (3, 0)-32-polyhedral links

(b) The *I* (3, 0)-32-polyhedral links derived from *I* (3, 4)-62-polyhedral links

5. Conclusions

Research on even tangles develops a new method to construct the novel interlocked cages based on Extended Goldberg polyhedra, which are 4-regular. The new kinds of interlinked links are effective complements for tabulating the link table. Each of the polyhedral links can exists in two mirror image forms, denoted *D* and *L*, and it is usually true that they are analogous to some encountered in chemistry and biology. In chemistry, the chiral molecule is partitioned into two homochirality classes, denoted *R* and *S*, Δ and Λ, etc. In biology, the viral capsid may be one of them and a new medicinal model is the other. Particularly, these polyhedral links have *I* symmetry and therefore are said to possess topological chirality. Hence, they provide some potential models for icosahedral capsids, which possess chirality. In addition, with the increase of the tangle number of *2n*, or the twist number of *n*, the polyhedral links will take place a class of non-isotopy transformation. These topological transformations satisfy the icosahedral symmetry group and show interesting mathematical properties and some possible bio-chemical significance. Covering the theoretical transformation may be one of ways in understanding the experimental synthesis of DNA catenanes.

Odd tangles, other building blocks of polyhedral links, will lead to more complex topological structures. The research of those constructions is of importance in understanding the molecular design of polehedral links from tangles and we shall discuss them in detail elsewhere.

Acknowledgements

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