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Topological transformation of dual polyhedral links

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Abstract

In this paper, the novel topology of Platonic polyhedral links is discussed on the basis of the graph theory and topological principles. This interesting problem of the dual polyhedral links has been solved by using our method of the 'sphere-surface-movement'. There are three classes of dual polyhedral links which can be explored: the tetrahedral link is self-dual, the hexahedral and octahedral link, as well as the dodecahedral and icosahedral link are dual to each other. Our results show that the duality of self-dual tetrahedral link is 'trivial', and the duality of hexahedral and octahedral link as well as dodecahedral and icosahedral link are 'nontrivial'. This study provides further insight into the molecular design and theoretical characterization of the new polyhedral links.

1. Introduction

As the interlinked architectures, topological links [1-8] are the new forms of molecular structures, from organic molecules to DNA. There have been many milestones in the development of syntheses of DNA polyhedral links including the DNA tetrahedron [9, 10], DNA cube [11, 12], DNA truncated octahedron [13], DNA octahedron [14], and DNA trigonal bipyramid [15]. Knot theory, a branch of topology, provides us a useful tool to research molecular catenanes and has made a connection with chemistry. For example, many polyhedral links have been constructed based on Goldberg polyhedra, carbon nanotubes, and some other novel polyhedra by Qiu and his co-workers [26-30]. Despite these successes, it is the very first time for investigating the duality of polyhedral links in chemical and natural world.

In geometry, duality means closely related relationships between two patterns, particularly, two polyhedra. If the centers of faces of one polyhedron are the vertices of the other, they are considered to be dual, which implies their symmetry groups coincide. A pair of dual polyhedra can be exchanged through dual operation: truncation along their edges or truncation of their vertex perpendicular diagonals. According to the dual theory, five Platonic polyhedra can be divided into three groups: two self-dual tetrahedrons, the hexahedron and octahedron, the dodecahedron and icosahedron, where the two latter groups are dual to each other [31]. However, polyhedral links are some forms more complex than polyhedra, because they can be transformed to each other not only by geometrical operations but also by topological changes, such as twisting, bending and stretching. Due to these particular topological properties, their dual relationships shall be more interesting and need further exploring. Describing it mathematically is a nice challenge!

To achieve our goals, we first use 'three-cross-curve and double-line covering' [32] to construct original polyhedral links, and then use a new method of 'sphere-surface-movement' as the dual transformation on the basis of topological principles. As a result, Platonic polyhedral links belong to six dual groups, in which three are left-handed and another three are right-handed. Among them, the tetrahedral link is self-dual, the hexahedral and dodecahedral link are dual to the octahedral link and icosahedral link, respectively. Moreover, duality is divided into 'trivial' and 'nontrivial' in physics. Thus, the self-dual relationship of tetrahedral links is considered to be 'trivial', and the other dual relationships between two different links are 'nontrivial'. More curiously, our research provides a new point of view for the molecular design and theoretical characterization of polyhedral links.

2. Dual polyhedral links

In graph theory, given a plane graph G, the medial graph $Med(G)$ is defined as the graph having as vertices the edges of G with two vertices adjacent if and only if they share a vertex and belong to a common face. If $Med(G) = Med(G^*)$, then G and G^* are dual [34]. It is easy to know that $Med(G)$ are all 4-valent. See Fig. 1.

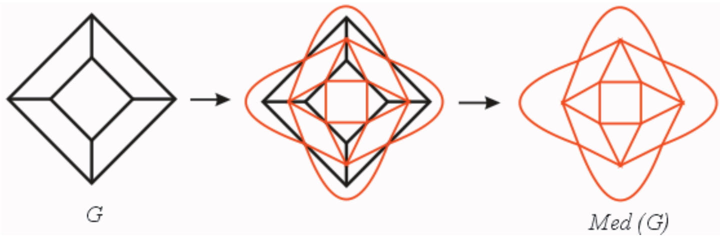

Fig. 1. The progress of a plane graph G changes to a medial graph $Med\ (G)$

In knot theory, there is a one-to-one correspondence between link diagrams and plane graphs [35]. From a projection of link L, a corresponding planar graph G can be created in the following way. First shade every other region of the link diagram so that the infinite outermost region is not shaded, then put a vertex at the center of each shaded region and connects with an edge any two vertices which are in regions that share a crossing. See Fig. 2.

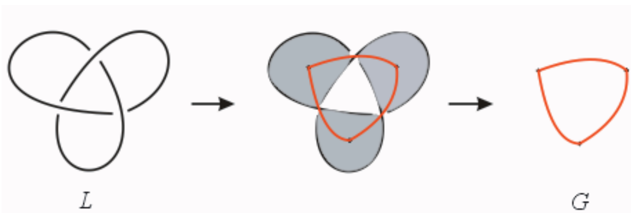

Fig. 2. The progress of a link L changes to a planar graph G

According to above basic concepts, we can define dual polyhedral links as follows:

(1) If polyhedra P_1 and P_2 are dual, then $Med\ (P_1) = Med\ (P_2)$;

(2) If $L\ (P_1)$ and $L\ (P_2)$ are two polyhedral links, then $G\ (L\ (P_1))$ and $G\ (L\ (P_1))$ are their corresponding planar graphs;

(3) If $G\ (L\ (P_1)) = Med\ (P_1)$ and $Med\ (P_2) = G\ (L\ (P_2))$, then $L\ (P_1)$ and $L\ (P_2)$ are a pair of dual polyhedral links.

3. Polyhedral links construction

In this section, the construction of polyhedral links is the foundation of future development of new dual links. The original polyhedral link is constructed by using a three-cross-curve to cover a vertex and using a double-line to cover an edge, then connecting the three-cross-curve with the double-line, respectively. This method is called ‘three-cross-curve and double-line covering’ and can only be used for 3–regular polyhedra. Thus, among five Platonic polyhedra, we can construct the corresponding tetrahedral link, hexahedral link, and dodecahedral link.

If using 4 three-cross-curve and 6 double-line as building blocks to cover 4 vertices and cover 6 edges, respectively, in the tetrahedron, and connecting the three-cross-curve with the double-line, then, it is surprising to get one interesting tetrahedral link (Fig. 3). The hexahedral link (Fig. 4) and dodecahedral link (Fig. 5) are constructed by the same process but different numbers of building blocks as the tetrahedral link. In general, if using 8 three-cross-curve and 12 double-line in the hexahedron, then the hexahedral link is obtained, and if using 20 three-cross-curve and 30 double-line in the dodecahedron, then it is surprising to discover a curious dodecahedral link (Fig. 5).

4. The topological transformation of dual polyhedral links

‘Sphere-surface-movement’ is such a manipulation that each component of polyhedral links continuously moves on the spherical surface after the link is transformed to a spherical surface through topological mapping. The continuous movement means that the manipulation, which can be achieved without cutting and joining, is topological. Applying this method to polyhedral links which we have constructed in section 3, three groups of dual polyhedral links are obtained.

In order to describe our ideas, for the example, the manipulation of ‘sphere-surface-movement’ for the tetrahedral link is shown in Fig. 3. First, transform the tetrahedral link in R^3 (Fig. 3(a)) to a spherical surface. Second, move 4 loops of the tetrahedral links (Fig. 3(b)) on spherical surface in direction, then an ‘intermediate’ (Fig. 3(d)) and the spherical surface

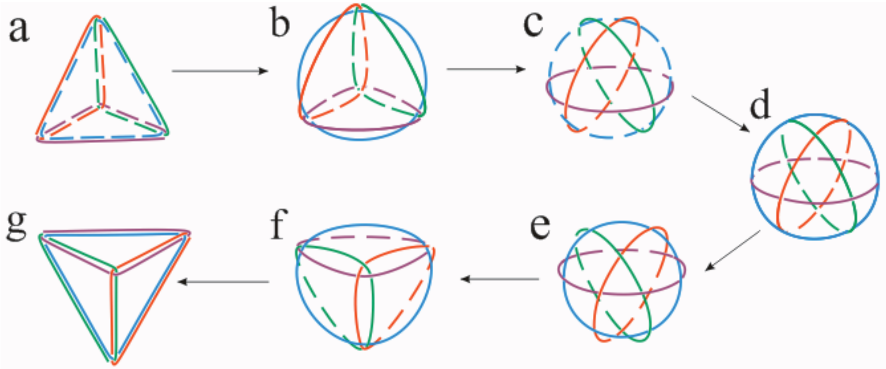

Fig. 3. The topological transformation of tetrahedral link

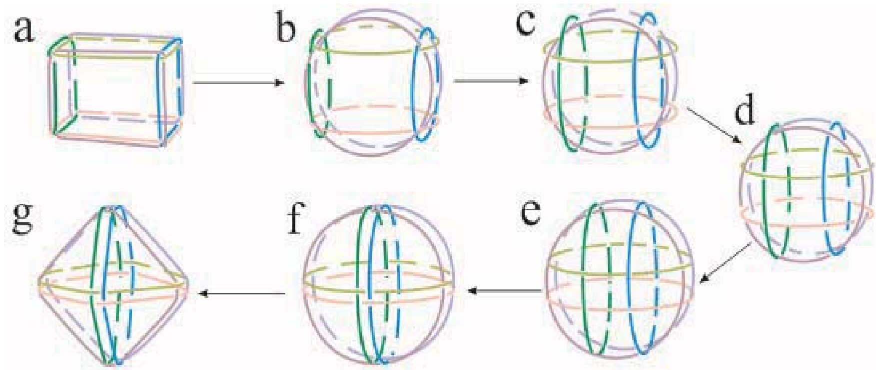

Fig. 4. The topological transformation of hexahedral link

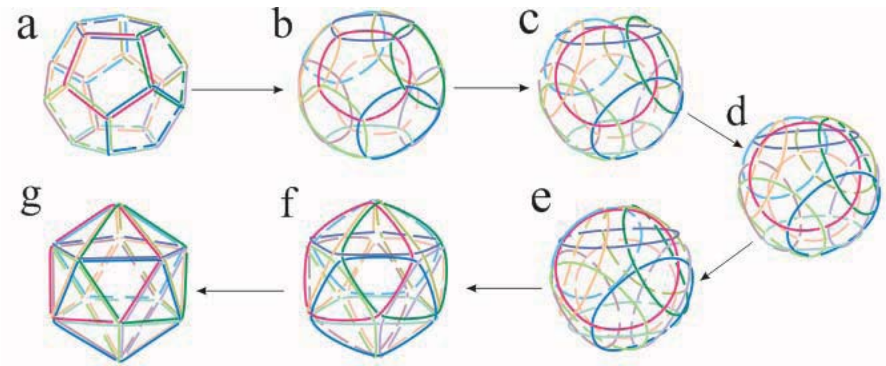

Fig. 5. The topological transformation of dodecahedral link

of a new tetrahedral link (Fig. 3(f)) emerge. Finally, the spherical surface of new tetrahedral link (Fig. 3(f)) is topologically deformed to the new tetrahedral link (Fig. 3(g)) in R^3. In the progress, we can obtain a new tetrahedral link from the original one; thus, the tetrahedral link is self-dual.

In contrast with the tetrahedral link, the topologically transformation from the hexahedral link (Fig. 4(a)) and dodecahedral link (Fig. 5(a)) to the octahedral link (Fig. 4(g)) and icosahedral link (Fig. 5(g)) are shown in Fig. 4 and Fig. 5, respectively. The octahedral link (Fig. 4(f)) and an 'intermediate' (Fig. 4(d)) can be generated by the oriented movement of 6 loops of the hexahedral link (Fig. 4(b)) on spherical surface. And then, the octahedral link in R^3 (Fig. 4(g)) is generated by topological mapping. It means that the hexahedral link and the octahedral link are dual. Similarly, the emergence of the icosahedral link (Fig. 5(f)) and an 'intermediate' (Fig. 5(d)) requires oriented movement of 12 loops of the dodecahedral link (Fig. 5(b)) on spherical surface. Topological transformation shows that the dodecahedral link and the icosahedral link are also a pair of dual polyhedral links.

The processes of 'sphere-surface-movement' for the tetrahedral link, octahedral link, and icosahedral link are shown in Fig. 3, 4, and 5. As a result, we can obtain the dual of such three polyhedral links: another tetrahedral link, the octahedral link, and the icosahedral link, respectively. In contrast with the tetrahedral link, four-cross-curve and five-cross-curve are building blocks, which are used to construct the octahedral link and icosahedral link, respectively. Thus, two new methods, 'four-cross-curve and double-line covering' (Fig. 6(a)) and 'five-cross-curve and double-line covering' (Fig. 6(b)), are developed for constructing polyhedral links for 4-regular and 5-regular polyhedra.

The octahedron has O_h symmetry group, and with vertices of degree 4. It is easy to see that its link, which is O symmetry, can be constructed by 6 four-cross-curve and 12 double-line through the method of 'four-cross-curve and double-line covering'. The polyhedron with I_h symmetry group has vertices of degree 5. Hence its link with I symmetry can be constructed by 12 five-cross-curve and 30 double-line through the method of 'five-cross-curve and double-line covering'.

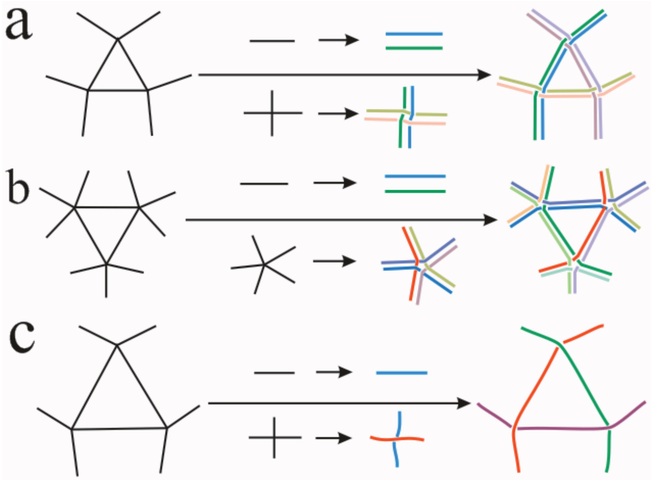

Fig. 6. Three new methods of constructing polyhedral links

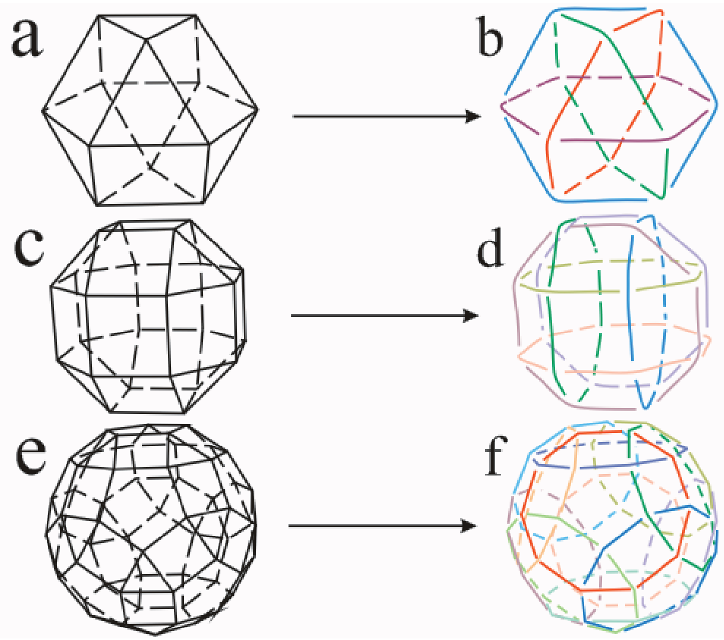

Fig. 7. Archimedean polyhedra and their links

In the process of addressing the duality of polyhedral links, three-cross-curves and double-lines are thereby changed into triangular and rectangular spaces. If the position of each loop is proper, the rectangular spaces change to square spaces, and three 'intermediates' (Fig. 3(d), 4(d), and 5(d)) emerge. In fact, using the method of 'cross-curve and single-line covering' (Fig. 6(c)), then three polyhedral links (Fig. 7(b), (d), and (f)), which correspond to three 'intermediates', can be constructed from Archimedean polyhedra (3 4 3 4), (3 4 4 4), as well as (3 5 3 5) (Fig. 7(a), (c), and (e)).

5. Discussion

The study of the topological process of dual polyhedral links, from Fig. 3 to Fig. 5, reveals three outstanding properties:

(1) A pair of dual polyhedral links has the same symmetry and chirality. In our work, the tetrahedral link (Fig. 3(a)), hexahedral link (Fig. 4(a)) and dodecahedral link (Fig. 5(a)) correspond to the 'sphere-surface-movement' of 4, 6, and 12 loops, respectively. During the progress of dual transformation, we assume each loop is infinitely flexible and cannot be broken during deformation. Hence it is not difficult to know that three groups of dual polyhedral links keep *T, O, I* symmetry, respectively. In addition, the chirality of dual polyhedral links is also kept. It means that we cannot turn the left-handed polyhedral link to its dual right-handed polyhedral link by a topological operation.

(2) Three groups of dual polyhedral links are classified into two types of duality. Physicists use the term 'duality' to describe theoretical models that appear to be different but can be shown to describe exactly the same physics, and are divided into 'trivial' and 'nontrivial'. There are three groups of polyhedral links: the tetrahedral link and another tetrahedral link; the hexahedral link and the octahedral link; the dodecahedral link and the icosahedral link. The first group of two tetrahedral links is self-dual, and both of them can be obtained by 'three-cross-curve' as building blocks. Therefore, it is 'trivial' because there are none of new forms has been presented in their dual translation. Such translation, which is the same as the translation between two different languages, brings no new insight. The second group contains the hexahedral link and the octahedral link, which are constructed by

'three-cross-curve' and 'four-cross-curve', respectively. The third group contains the dodecahedral link and the icosahedral link, which are constructed by 'three-cross-curve' and 'five-cross-curve', respectively. Although their topological characteristics and symmetry remain unchanged, new methods of constructing polyhedral links and new polyhedral frames appear; hence these two groups of dual polyhedral links belong to 'nontrivial'. The process is similar with the transmutation between water and ice. We notice quite easily that the self-dual of tetrahedral link is 'trivial'; whereas, the duality of hexahedral link and octahedral link, as well as the duality of dodecahedral link and icosahedral link belong to 'nontrivial'.

(3) The construction of dual polyhedral links is alterative. Starting from the hexahedral and hexahedral link with 'three-cross-curve and double-line covering', the structures of octahedral and icosahedral link with 'four-cross-curve and double-line covering' and 'five-cross-curve and double-line covering' are obtained, respectively. As we known, the transformations are all topological, so 'three-cross-curve' can be transformed into 'three-cross-curve' and 'five-cross-curve', and vice versa. It means that the construction of dual polyhedral links is alterative.

6. Conclusions

Duality is a fundamental concept that underlies almost all natural phenomena. Roughly speaking, the duality is the product of the interaction that takes place between the paired components of an elementary system [36-38]. Research on Platonic polyhedral links develops a new form of duality on the topological spaces. It is represented as follows: the tetrahedral link is self-dual; the hexahedral link and dodecahedral link are dual to the octahedral link and icosahedral link, respectively. Thus, the method of the 'sphere-surface-movement' is a new topological dual operation in contrast with truncation in geometry. The basic investigation of dual polyhedral links enriches the theoretic characteristics of these novel structures.

Topological analysis indicates that duality preserves symmetry and chirality in dual polyhedral links. It is not difficult, intuitively, at least, to see that the left-handed link and right-handed link are distinct. Especially, in the natural world, it is true that one of them is the virus capsid and the other may be a medicinal model. Furthermore, considering of the handedness of polyhedral links, the result of 'sphere-surface-movement' is hence six groups of dual polyhedral links existing in ten Platonic polyhedral links. Three groups are left-handed and others are right-handed. How to find a new method to implement dual transformation with the reversal of handedness is still one of the biggest challenges.

Further, two types of duality, 'trivial' and 'nontrivial' are obtained. The 'trivial' links employ the same method for constructing polyhedral links, whereas the 'nontrivial' links use two different methods as 'four-cross-curve and double-line covering' and 'five-cross-curve and double-line covering' to construct polyhedral links. These two methods correspond to polyhedra with vertices of degree 4 and 5, respectively. Now we are ready to achieve some nice drawings using simple constructions! It is important to remember that they enrich the method of constructing polyhedral links. Additionally, these new forms are the foundation of future development of new products and processes, so that synthetic chemists and biologists are able to test and develop their synthetic strategies.

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References

[1] C.C. Adams, *The Knot Book: An Elementary Introduction to the Mathematical Theory of Knots,* W.H. Freeman & Company, New York, 1994.

[2] P.R. Cromwell, *Knots and Links,* Cambridge University Press, Cambridge, 2004.

[3] S. Jablan, R. Sazdanovic, *Linknot- Knot Theory by Computer,* World Scientific, Singapore, 2007.

[4] K. Mislow, A commentary on the topological chirality and achirality of molecules, *Croat. Chem. Acta.* **69** (1996) 485-511.

[5] K. Mislow, C.Z. Liang, Knotted structures in chemistry, biochemistry, and molecular biology, *Croat. Chem. Acta.* **69** (1996) 1385-1403.

[6] J.P. Sauvage, C.D. Buchecker (Eds.), *Molecular Catenanes, Rotaxanes and Knots,* Wiley – VCH, New York, 1999.

[7] W.R. Taylor, K. Lin, Protein knots: A tangled problem, *Nature* **421** (2003) 25.

[8] C. Helgstrand, W.R. Wikoff, R.L. Duda, R.W. Hendrix, J.E. Johnson, L. Liljas, The refined structure of a protein catenane: the HK97 bacteriophage capsid at 3.44 A resolution, *J.Mol.Biol.* **334** (2003) 885-899.

[9] R.P. Goodman, R.M. Berry, A.J. Turberfield, The single-step synthesis of a DNA tetrahedron, *Chem. Commun.* **12** (2004) 1372-1373.

[10] R.P. Goodman, I.A.T. Schaap, C.F. Tardin, C.M. Erben, R.M. Berry, C.F. Schmidt, A.J. Turberfield, Rapid chiral assembly of rigid DNA building blocks for molecular nanofabrication, *Science* **310** (2005) 1661-1665.

[11] J.H. Chen, N.C. Seeman, Synthesis from DNA of a molecule with the connectivity of a cube, *Nature* **350** (1991) 631-633.

[12] N.C. Seeman, DNA in a material world, *Nature* **421** (2003) 427-431.

[13] Y. Zhang, N.C. Seeman, Construction of a DNA-truncated octahedron, *J. Am. Chem. Soc.* **116** (1994) 1661-1669.

[14] F.F. Andersen et.al., Assembly and structural analysis of a covalently closed nano-scale DNA cage, *Nucl. Acids Res.* **36** (2008) 1113–1119

[15] C.M. Erben, R.P. Goodman, A.J. Turberfield, A self-assembled DNA bipyramid, *J. Am. Chem. Soc.* **129** (2007) 6992-6993.

[16] P.G. Mezey, Tying Knots Around Chiral Centres: Chirality Polynomials and Conformational Invariants for Molecules, *J. Am. Chem. Soc.* **108** (l986) 3976-3984.

[17] E. Flapan, *When Topology Meets Chemistry – a Topological Look at Molecular Chirality*, Cambridge University Press, Cambridge, 2000.

[18] W.-Y. Qiu, H.-W. Xin, Molecular design and topological chirality of the Tq-Mobius ladders, *J. Mol. Struct*. (THEOCHEM) **401** (1997) 151-156.

[19] W.-Y. Qiu, H.-W. Xin, Molecular design and tailor of the doubled knots, *J. Mol. Struct*. (THEOCHEM) **397** (1997) 33-37.

[20] W.-Y. Qiu, H.-W. Xin, Topological structure of closed circular DNA, *J. Mol. Struct.* (THEOCHEM) **428** (1998) 35-39.

[21] W.-Y. Qiu, H.-W. Xin, Topological chirality and achirality of DNA knots, *J. Mol. Struct.* (THEOCHEM) **429** (1998) 81-86.

[22] W.-Y. Qiu, Knot theory, DNA topology, and molecular symmetry breaking, in: D. Bonchev, D.H. Rouvray (Eds.), *Chemical Topology – Applications and Techniques*, *Mathematical Chemistry Series, Vol.6,* Gordon and Breach Science Publishers, Amsterdam, 2000, pp. 175–237.

[23] J.S. Siegel, Chemical topology and interlocking molecules, *Science* **304** (2004) 1256-1258.

[24] C. Liang, K. Mislow, Topological chirality of proteins, *J. Am. Chem. Soc.* **116** (1994) 3588-3592.

[25] J. Rudnick, R. Bruinsma, Icosahedral packing of RNA viral genomes, *Phy. Rev. Lett.* **94** (2005) 038101

[26] W.-Y. Qiu, X.-D. Zhai, Molecular design of Goldberg polyhedral links, *J. Mol. Struct.* (THEOCHEM) **756** (2005) 163-166.

[27] G. Hu, X.-D. Zhai, D. Lu, W. -Y. Qiu, The architecture of platonic polyhedral links, *J. Math. Chem*. 2008 (DOI 10.1007/s10910-008-9487-z)

[28] Y.-M. Yang, W.-Y. Qiu, Molecular design and mathematical analysis of carbon nanotube links, *MATCH Commun. Math. Comput. Chem.* **58** (2007) 635-646.

[29] G. Hu, W.-Y. Qiu, Extended Goldberg polyhedral links with even tangles, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 737-752.

[30] G. Hu, W.-Y. Qiu, Extended Goldberg polyhedral links with odd tangles, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 753-766.

[31] A.K. van der Vegt, *Order of Space*, Vereniging voor Studie-en Studentenbelangen te Delft, 2001.

[32] W.-Y. Qiu, X.-D. Zhai, Y.-Y. Qiu, Architecture of platonic and archimedean polyhedral links, *Sci. China Ser. B-Chem.* **51** (2007) 13-18.

[33] M.J. Duff, The theory formerly known as strings, *Sci. Amer.* **278** (1998) 64-69.

[34] D. Archdeacon, J. Siran, M. Skoviera, Self-dual regular maps from medial graphs, *Acta. Math. Univ. Comenianae.* **1** (1992) 57-64.

[35] C.C. Adams, *The Knot Book*, W. H. Freeman and Company, New York, 1994, pp. 51-55.

[36] M. Mukerjee, Explaining everying, *Sci. Am.* **274** (1996) 88-94.

[37] B.G. Englert, M.O. Scully, H. Walther, The duality in matter and light, *Sci. Am.* **271** (1994) 86-92.

[38] E. Bergshoeff, M. de Roo, D-branes and T-duality, *Phys. Lett. B.* **380** (1996) 265-272.