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A Survey on Mathematical Models for DNA Polyhedra

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Abstract

Mathematical models for DNA polyhedra represent important and imminent challenges for mathematical chemistry. In recent years, there has been growing interest in applying knot theory and polyhedral topology to meet this challenge. The knot approach transforms a DNA polyhedron into a polyhedral link by connecting vertices and edge building blocks. Thus, it is possible to describe DNA polyhedra by understanding the construction method of polyhedral links, and studying their knot invariants and relationships. As an alternative mathematical mode, DNA cages have also proved to be useful tools for describing DNA polyhedra, in terms of topological graph analysis and the molecular design based on octet truss. This minireview aims to summarize recent progress in these two kinds of mathematical models for DNA polyhedra, and hope to arouse broader interests in this area for both biochemists and mathematicians.

1. Introduction

Chemical topology [1], a recently blossoming area in mathematical chemistry, is concerned with topologically nontrivial species, such as catenanes and knots. When DNA meets chemical topology give birth to a new field of structural DNA nanotechnology [2]. Owing to the helical structure and Watson-Crick base pairing rules, DNA can be programmed to self assemble into a number of nanoarchitectures with connectivity of polyhedra. In the seminal paper, Seeman [3] firstly used branched DNA molecules to construct the cube. Since then, a rich variety of simple DNA polyhedra including tetrahedron [4], octahedron [5] and truncated octahedron [6], and more complex DNA polyhedra including dodecahedron [7] (Fig. 1b), icosahedron [8], and buckyball [9] have now been assembled, as shown in Fig. 1, which may have potential applications in drug delivery. The interest in these species is rapidly increasing not only for applications but also for their state-of-the-art architectures.

These DNA nano-constructions now have changed our understanding of the shape of polyhedra, in which each vertex represents a DNA multi-arm junction, and each edge is made of double-helix or quadruplex-helix DNA strands. The current mathematical treatments to address these structural puzzles are based on knot theory coupled with polyhedral topology. Polyhedral links [10], their construction rules, knot invariants and Euler relationship were considered to be the first step to understanding the structural principle of DNA polyhedra. DNA cages [11], based on topological graph theory, have also impelled a search for an even deeper understanding of structural DNA nanotechnology. Our paper attempts to provide an overview of current research of these two mathematical models for DNA polyhedra, where there is interplay between knot theory and polyhedral topology.

The next section is devoted to some basic concepts of knot theory and the mathematics of polyhedra, and their relevance to chemistry. A variety of properties of polyhedral links, from construction method, to knot invariants and their Euler relationships, will be investigated in Sect.3, whereas the other type of mathematical model of DNA cages will be discussed in Sect. 4. For the detail mathematical definition and background, there is a need to refer to other specialized papers or monographs [12, 13]. Herein, we just start with necessary mathematics.

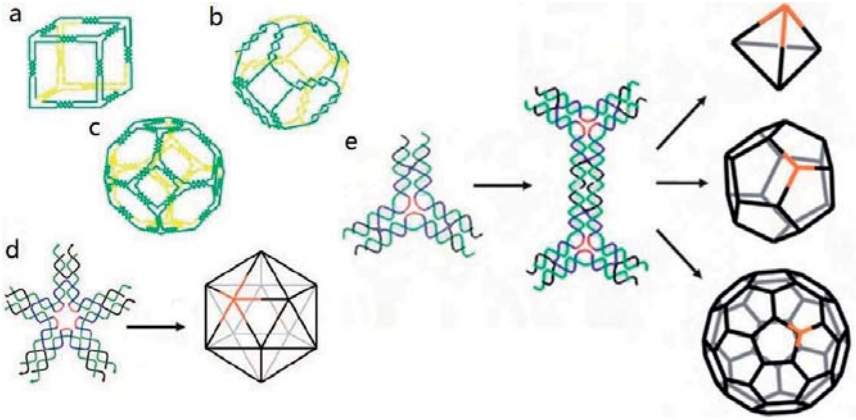

Fig. 1. Three-dimensional DNA polyhedra. (a) A DNA cube, (b) a DNA octahedron and (c) a DNA truncated octahedron. (d) A DNA icosahedron assembled from and five-point-star motifs and (e) a tetrahedron, a DNA dodecahedron and a DNA buckyball assembled from three-point-star motifs.

2. Fundamentals of knot theory and polyhedral topology

2.1 Knot theory in chemistry

Knot theory studies the embedding of one topological space into another, for example, the placement of a circle into three-dimensional space [13]. The central problem in knot theory is thus to classify these different topological objects, with the help of various kinds of knot invariants. These invariants could either be crossing number, genus, braid index, and knot polynomials, etc.

Now, it is well known that molecular knots and links are common examples in chemistry, biochemistry and molecular biology [14]. Moreover, knot theory has been successfully applied to understand DNA recombination process and protein knotted structures. As a promising development, the tangle topological approach was first proposed by Ernst and Sumners [15] to detect enzyme mechanisms, and soon thereafter determine various features of DNA topology and biological reactions [16]. Although knotted proteins are of less common occurrence, knot theory may help us to go deeper into protein knots characterization and the understanding of their biological role in this developing area [17]. Recent advances include studying descriptors for the analysis of protein symmetries and proteins classification, and

developing algorithms to detect knots in proteins.

Chirality is at the very heart of chemistry. In knot theory, chirality can be detected by knot invariants of polynomials. To this end, two important chirality-sensitive polynomials have been proposed. Vaughan Jones introduced the Jones polynomial in 1984 [18], and soon after it was generalized by the HOMFLY polynomial [19]. Despite these mathematical results, chemists have also tackled this chemistry oriented problem. By transforming a molecule to the corresponding knot, Mezey [20] developed a knot-theoretical polynomial description of the chirality of molecules containing an arbitrary large number of chiral and achiral carbon centers. In addition, a method for detecting topological chirality and achirality of links has been developed by Liang and Mislow [21], based on the concept of U-polynomials.

2.2 Polyhedral topology in chemistry

Polyhedral structures are basic markers of space, which have attracted scientists' attentions due to their shapes, symmetries and mathematical properties [22]. A large number of polyhedral molecules synthesized and found both in laboratory and nature have led theoretical chemists to explore their structural characteristics [23–25], form geometry to topology. Owing to their high symmetry, Platonic polyhera and Archimedean polyhedra have deserved special attention. Platonic polyhera, as the best known family of polyhedra, are characterized by having all faces formed identical, all vertices and edges equivalent. Archimedean solids, another important type of semiregular polyhedra, are resulted from Platonic solids by truncating or snubbing operation.

The fundamental equation governing polyhedral topology is Euler's formula [26]:

$$V + F = E + 2$$

where V, F and E are the respective total numbers of vertices, faces and edges of the polyhedron. Separate relations may also be established between pairs of these structural elements. As an example, let n_i denote the degree of the i-th vertex, and let p_j denote the number of sides to face j, with $n_i \geq 3$ and $p_j \geq 3$. Then, we have:

$$\sum_{i=1}^{V} n_i = \sum_{j=1}^{F} p_j = 2E$$

As a matter of fact, Euler's formula not only describes polyhedral topology, but also provides a profound characteristic of knotted structures. According to the formula, one can calculate Euler characteristics of a knot. This quantity simplifies the knot classification problem by assigning a topological surface to a knot. Each different knot will embedded as a boundary of a certain surface, which is characterized by Euler characteristic.

In terms of polyhedra, duality means the centers of faces of one polyhedron are the vertices of the other. Among the Platonic solids, for the example, the cube and the octahedron are duals of each other, so are the icosahedron and the dodecahedron, while the dual of a tetrahedron is just another tetrahedron. The dualization process shows that edge number and symmetry are preserved, implying a transformational relationship between polyhedra, which might be of considerable importance in chemistry.

3. DNA polyhedral links

Polyhedral links are mathematical models of DNA polyhedra, which regard DNA as a very thin string [10]. A polyhedral link is an interlinked and interlocked architecture that is obtained from a polyhedral graph, by using tangled structures to replace its vertices and edges. It is worth noting that polyhedral link models for DNA polyhedra all are alternating, which means their crossings alternate between over and undercrossings along one strand.

3.1 Construction methods

The beginning of study on polyhedral links was inspired by the remarkable discovery of topologically linked protein catenane in HK97 bacteriophage [27]. It was found by Qiu *et al*. [28] that these novel structures could be theoretically constructed through "three-cross-double-line covering" and "*n*-crossover-double line covering" methods, as shown in Fig. 2a. We call this type of links as *crossed polyhedral links*. The geometry of Goldberg polyhedra is a good start for constructing polyhedral links. Replacing each vertex and edge of Goldberg polyhedra with three-crossover and double line respectively, a member of Goldberg polyhedral links is constructed. Interestingly, Goldberg polyhedral links usually have I symmetry while corresponding Goldberg polyhedra have I or I_h symmetry. This means symmetry breaking occurs while constructing Goldberg polyhedral links.

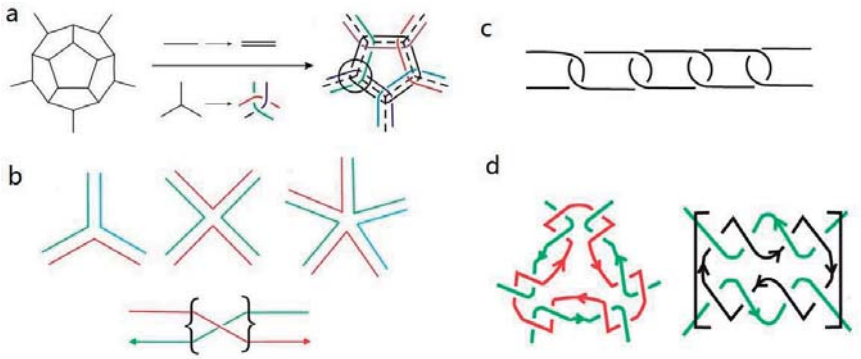

Fig. 2. (a) The construction method of crossed polyhedral links. The building blocks for (b) tangled polyhedral links, (c) cycle-crossover polyhedral links and (d) star polyhedral links.

The success construction of Goldberg polyhedral links evokes mathematicians and chemists to generalize construction methods of polyhedral links. The same construction method has also been used to construct polyhedral inks based on Platonic and Archimedean polyhedra [29]. 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. In order to overcome the vertices degree problem, a more general approach of "*n*-branched curves and *m*-twisted double-lines covering" (Fig. 2b) was proposed [30]. In this approach, two types of basic building blocks for polyhedral links are needed. One is an *n*-branched curve designed to replace the vertex of a polyhedron, where *n* is equal to the vertices degree. The other is an *m*-twisted double-line, which is proposed to replace the edge of a polyhedron.

Another way of generalizing construction method is borrowed from classical knot theory. This method, first described by our earlier works [31, 32], was to use tangles to replace vertex structures of a polyhedra. A tangle in knot theory, as some examples like *m*-twisted double-lines, is two strands surrounded by a circle and twisted around each other. Since a tangle has four branches at ends, it is an ideal building block for the construction of knots and links on four-degree polyhedra. In order to obtain such polyhedra, we first constructed two types of extended Goldberg polyhedra, namely stretch-extended Goldberg polyhedra and

rotate-extended Goldberg polyhedra. Then, with the help of tangle theory, we constructed a series of stretch-extended Goldberg polyhedral links and rotate-extended Goldberg polyhedral links. Interestingly, symmetry breaking also occurs on these extended Goldberg polyhedral links. The type of polyhedral links constructed by this method was called *tangled polyhedral links*. It further illustrated that two additional types of polyhedral links, named *cycle-crossover polyhedral links* [33] (Fig. 2c) and *star polyhedral links* [34] (Fig. 2d), have also been constructed, which are covered by the currently existing construction theories.

It should be pointed out that, the construction of polyhedral links has learned much from polyhedral topology. Lu *et al.* [35] found the duality also exits in polyhedral links, by the method of "sphere-surface-movement". Similar with the duality in polyhedra, it was shown that the tetrahedral link is self-dual, the hexahedral and octahedral link, as well as the dodecahedral and icosahedral link are dual to each other. Fig. 3 shows the topological transformation between two dual polyhedral links. This transform also implies three new construction methods: "four-cross-curve and double-line covering", "five-cross-curve and double-line covering" and "cross-curve and single-line covering". As we known, the symmetry is kept for dual polyhedra. However, the chirality is kept if dual polyhedral links are constructed by *E*-tangles, otherwise is reversed for *O*-dual links [36].

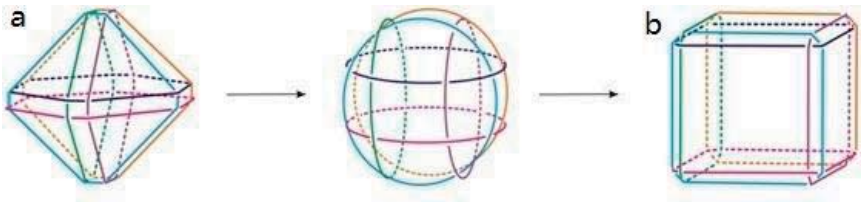

Fig. 3. The dual transformation between (a) an octahedral and (b) the corresponding hexahedral link.

Jablan *et al.* [37, 38] proposed two kinds of construction method, and used low symmetry pyramids and prisms as basic construction skeleton. The first one, generalized Jaeger construction, is based on the generalized construction of middle graphs, which is surprisingly same with "*n*-branched curves and *m*-twisted double-lines covering". The other one, generalized dual Jaeger construction, is based on the truncation and doubling of edges. For

example, as shown in Fig. 4, the polyhedral link is obtained by generalized Jaeger construction based on 3-prism graphs. For extension, they [39] investigated the possibility of forming polyhedral links via templating on different surfaces, such as graphs K_5 and $K_{3,3}$. The results suggested that virtual knot theory offers a useful tool to study molecular knots and links with more complexity. Finally, Jablan *et al.* [40] have tried to unify all the existing construction methods of polyhedral links, by introduce mid-edge construction, cross-curve and double-line covering, and edge doubling constructions. Thus, they fulfilled the first step toward a unifying theory of polyhedral links.

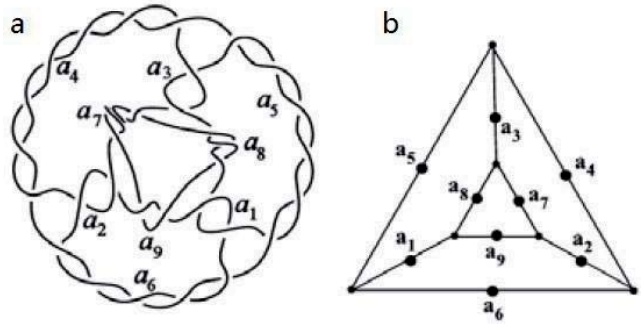

Fig. 4. (a) The 3-prism link is generated by (b) the corresponding graph by the generalized Jaeger construction [37].

3.2 Knot invariants

One of the central and most intriguing questions in mathematical theory of knot is how to effectively classify different knots. Knot invariants have turned out to be one of the successful tools to characterize different knots, and thus they can be used as molecular descriptors to describe the various configurations of large molecules that have non-planar graphs. So far, standard knot invariants including genus, braid index and different knot polynomials have been discussed. Among them, genus and braid index may be two most important invariants for polyhedral links. Genus is the basic topological feature of a surface, which denotes the number of holes going through the surface. The braid index of an oriented link is the minimum number of strings among all closed braid representatives for the given oriented link. Apart from its mathematical relevance, they are also of substantial interest to modern

chemistry and biochemistry. For examples, genus has been lent to guide the molecular design [41] and classify RNA structures [42], whereas representing knotted hydrocarbon complexes as closed braids can facilitates the study of their properties [43].

In [44], we proved that genus of all tangled polyhedral links are zero, it means that Seifert surfaces of these links are homeomorphic to spheres with a set of discs removed. If consider genus as a complexity measure, it is trivial for tangled polyhedral links. For a crossed polyhedral link L based on the n-pyramid p, Cheng *et al.* [45] computed its genus $g(L)$ to be n-2 if n is divisible by 3, otherwise to be n-1, where n denotes the maximum degree of P. For this case, genus shows an effect complex measurement for polyhedral links. The braid index for the four simple types of tangled polyhedral links, two more complicate types of cycle-crossover polyhedral links and star polyhedral links were all calculated. In particular, Cheng *et al.* [46] calculated $b(L)$ for four simple types of tangled polyhedral links, which are equal to $\frac{C(L)}{2}+1$. Cheng *et al.* [47] and Liu *et al.* [48], independently, proved that $b(L)$ of two complicated polyhedral links show the same value. The results means that braid index for polyhedral links are only depend on crossing number, showing a simple metric for complexity.

On the other hand, polynomial invariants have turned out to be one of the successful tools to characterize different knots. The Jones polynomial is an invariant of an oriented knot or link which assigns to each oriented knot or link a Laurent polynomial in the variable $t^{\frac{1}{2}}$ with integer coefficients, which can distinguish many links from their mirror images and thus has many chemical and physical applications. Jones polynomials of many types of knots have been already calculated, such as 2-bridge knot, prezel links, and tour links and so on. However, for polyhedral links, it is generally difficulty to compute the Jones polynomial. Cheng *et al.* [33], for the first time, computed Jones polynomials for cycle-crossover polyhedral links via the Tutte polynomial of the 1-skeleton of the polyhedron. Jin *et al.* [49, 50] have given some new results of Jones polynomials for all the tangled polyhedral links, by trying to unify the construction based on edge covering, vertex covering, and mixed edge and vertex covering. It's worth noting that the component number of a link can be deduced from its Jones polynomial.

As the generalization of Jones polynomial, the HOMFLY polynomial is another powerful polynomial invariant, which is closely related to many other invariants, including genus and braid index. One interesting application is that the HOMFLY polynomial has been recently used to topological analysis of knotted proteins [51]. In 2009, Jin *et al.* [52] calculated the HOMFLY polynomials for tangled polyhedral links with even tangles. In the mean time, Liu *et al.* [53] have also got the results of HOMFLY polynomials for four types of even tangled polyhedral links. Since then, Liu *et al.* [54, 55] further generalized this methodology to a family of nearly arbitrary polyhedral links and odd tangled polyhedral links. Therefore, the topological framework for the computation of HOMFLY polynomials of polyhedral links is obtained.

3.3 Euler's formula

The study of knot invariants for polyhedral links opens a door to theoretically describe the DNA polyhedra by molecular descriptors, but the stereo-chemical control of these curious objects is still in its infancy. Therefore, it would greatly benefit from clear theoretical models which express the relationships between the constituent descriptors, much in the same way as Euler's formula has done for the classical polyhedra.

After experiencing the exotic kingdom of DNA polyhedral links, one must be confused or even lost his way. Complexity increases in both structural diversity and tedious polynomial formula. The power of mathematics, however, is to summarize the complicated natural phenomena in the most concise and elegant way. Therefore, one may ask what is the basic principle that determines complexity and diversity of DNA polyhedra? Actually, the question is not trivial at all. Hu *et al.* [34] has discovered a beautiful equation for DNA polyhedra: $s + \mu = c + 2$, where s defines the number of Seifert circles, μ is the number of components, and c is the number of crossings. The form of this elegant equation is reminiscent of Euler's famous formula on polyhedra, i.e. $V + F = E + 2$. We called this equation as the new Euler's formula for DNA polyhedra, with its Euler characteristic equals 2, which detects the topological characteristics including connectedness, holes, and twistedness of polyhedral links.

However, the new Euler's formula is too restrictive to describe DNA polyhedra, because it just consider polyhedral links whose all edges contain even half-twists. It is not difficult,

intuitively at least, to conclude that the genus of these kinds of DNA polyhedra equal zero, *i.e.* they are restricted to a surface homeomorphic to a sphere. More recently, Euler's theorem can be easily extended to DNA polyhedra embedded in torus or surfaces with higher genus. On this basis, Li *et al.* [56] put forward the concept of the new Euler characteristic, $\lambda = \mathrm{s} + \mu - c,$ to describe the tangled polyhedral links with both even and odd twists. Li *et al.* [57] have also investigated the possible forms of Euler's formula for crossed DNA polyhedral links.

Euler's formula characterizes basic property of a polyhedron, while this new formula on polyhedral links depicts math under a polyhedral links. The quantities in the formula describe the most important properties in DNA polyhedra. As constructed in laboratory, DNA polyhedra are consisted of several DNA strands interlinked through tangles or crossings. Thus, the number of DNA strands and crossings are vital parameters in DNA nanoconstruction. Under the guidance of this formula, chemists may largely zoom in the possible synthetic targets for DNA polyhedra. This is the direct implication of the new Euler's formula on DNA polyhedra. On the other hand, because of the vital role of the number of Serfeit surface, it is still possible to explore the field, in such an extent that enumerating topological combinatorics of different invariants. As one might imagine, the new Euler's formula will bridge different patches of DNA topology together and produce an integrated view of DNA polyhedra.

4. **DNA cages**

Based on topological graph theory, a novel model of DNA cages was proposed by Janska *et al.* [58], in which they consider a DNA polyhedron as a thickened graph. More strictly speaking, DNA cages are topologically embedded into orientable thickened graphs as deformation retracts. Such thickened graphs are compact orientable 2-dimensional surfaces constructed out of thickened *n*-junctions (vertices) and strips (edges) glued together. Thus, the number of boundary components for the thickened graph corresponds to the number of single stranded DNA molecules in the cage.

As DNA structures made of single circular DNA strand can be potentially easier to amplify, clone and in general use in laboratory experiments, it is of interest and particularly important to investigate the minimal number of single stranded DNA molecules needed for a

cage. Mathematically, it presents a fundamental question in topological graph theory. Given a target graph, what is the minimum number of *K*-armed branched junction or circular DNA molecules that must be designed to create the graph?

Janska and Saito [58] have investigated maximum and minimum numbers of boundary components and how this number changed in terms of recombinations or edge additions. In addition, they showed the change of component number also relates to some computational results, such as genus and Euler characteristics. In their further works, they extended this research to derive blueprints for the putative organization of DNA cages with icosahedral symmetry. Two building blocks are needed for the design of a DNA cage, one is the initial data and the other is thickened *n*-junctions: three-junctions for a dodecahedron, whilst four-junctions for an icosidodecahedron requires and five-junctions for an icosahedron. Jonoska and Twarock [11] have proved that a dodecahedral cage can be realized in terms of only two circular DNA molecules (Fig. 5a), by discussing four types of vertex configurations. Grayson *et al*. [59] and Jonoska *et al.* [60], respectively, demonstrated that minimal numbers of circular DNA molecules both are two for an icosidodecahedral cage (Fig. 5b) and an icosahedral cage (Fig. 5c).

On the other hand, the octet truss provides alternative geometric avenues for constructing and analyzing DNA cages. Octet truss, developed by R. Buckminster Fuller, fills three-space with regular tetrahedra and octahedra. It has been proved that octet truss can help the arrangement of phenylene ethynylene to realize hydrocarbon links [40]. In the context of DNA cage, Girard *et al.* [61] and Ellis-Monaghan *et al.* [62] have referred to this method as an accurate geometric framework for branched DNA junction molecule assembly. They found that just one or two tile types of branched junctions are needed to construct DNA Platonic and Archimedean cages embedded in the octet truss. For examples shown in [61], a tetrahedron, a truncated tetrahedron, and a truncated octahedron can be constructed with a minimum of two tiles, whereas an octahedron and a cuboctahedron can be constructed with a minimum of one tile types.

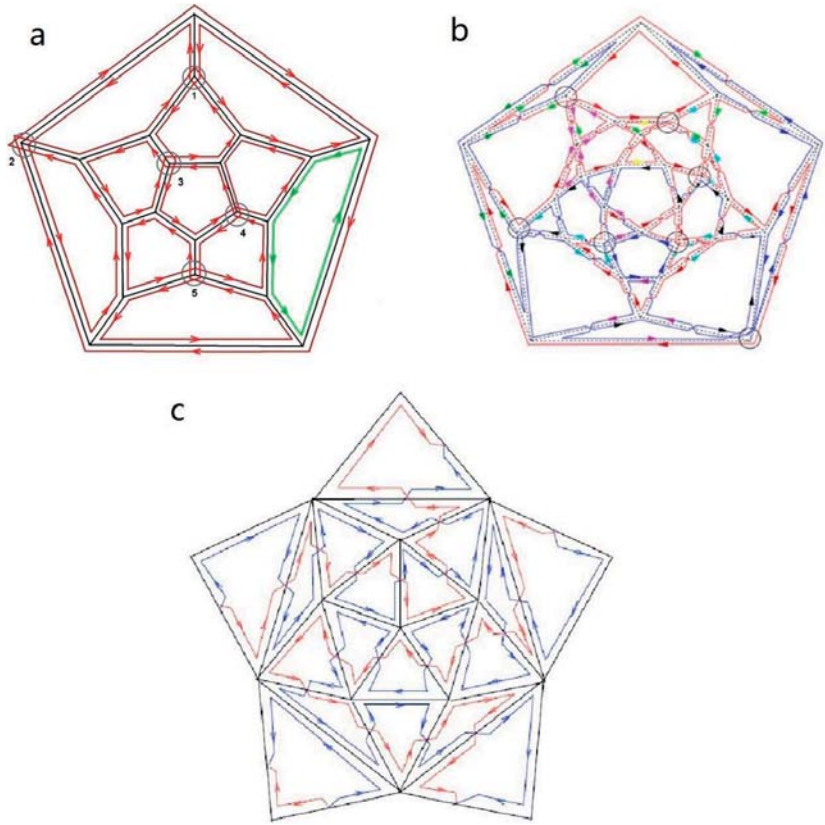

Fig. 5. (a) A dodecahedral [11], (b) an icosidodecahedral [61] and (c) an icosahedral [62] cage constructed with two DNA strands.

The study of the DNA cages, from topological graph theory to octet truss, reveals many opportunities and challenges both for mathematicians and experimental scientists:

(1) Although several mathematical models for DNA polyhedra have been pioneered, a more elegant and comprehensive general mathematical framework is need to be developed. In fact, Klavzar et al. [63] have realized these problems and tried their efforts to this area, such as the stable tracing model was proposed.

(2) The investigation of blueprints for the organization of the cages with minimal number of single DNA strands may suggest possible targets for experimental scientists and assist in their experimental realization. In the meantime, we have calculated that these blueprints

for DNA cage are embedded on surfaces with high genus, which also builds a rich treasure house for chemical investigation.

5. Concluding remarks and perspectives

With recent development in structural DNA nanotechnology, the application of knot theory and polyhedral mathematics to chemical topology has gained renewed interest. Two mathematical models of polyhedral links and DNA cages based on topological graph theory have been proposed and proved to be powerful ways to unravel the structural secrets of DNA polyhedra. Research on polyhedral links develops novel methods by the exploration of the systematic construction and transformation methods, the computation of different knot invariants, including genus, braid index and knot polynomials to describe their complexity and detect their chirality, the clear elucidation of relationships between knot invariants. The major endeavor of DNA cages is tried to derive all the blueprints of DNA polyhedra, with the help of topological graph analysis and the molecular design based on octet truss.

At the moment, however, there are many open problems appeared in the area of mathematical models for polyhedral links:

A systematic comparison and analysis of different construction methods is a task of the future. Re-analysis of the construction may give us deeper understanding of topological transformation between DNA polyhedra and their underlying chemical and biological processes.

The computation of more effective knot invariants and make them related to physico-chemical properties of DNA polyhedra. This not only provides rigorous descriptors to quantify the geometry and topology of DNA polyhedra, but also paves the way to the design of intrinsically novel structures.

A more refined analysis of DNA cages is still needed. In comparison with knot theory, graph theory shows a relative new tool and may be means a more surprise direction in structural DNA nanotechnology, such as Pólya's theorem has been applied to the enumeration problem of polyhedral links [64,65].

The potential application of these mathematical models has not been extensively explored so far. We have expected that the use of polyhedral links to characterize the recombinase regulation and controlling mechanisms for DNA polyhedra [66]. DNA cage models have also

been expected to uncover the genome packaging organizations in some viruses [67, 68].

In any event, we are at the very beginning of the understanding of structures for DNA polyhedra, as well as of the elucidation of their biological mechanism. Therefore, we hope this review will call attention for more innovative studies related to this area in the near future.

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