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Blueprints of the DNA Archimedean Polyhedra with Minimum Component Number

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Abstract

DNA has emerged as a versatile material for constructing functional nanostructures with specific topological arrangements, making it highly desirable for synthesizing of DNA nanostructures using minimal components. In this study, we propose a novel approach to fabricate polyhedra using the fewest possible components and investigate the roles played by different components. Our results reveal that even-sided polygon components are composed of subunits distributed contiguously or alternately, while odd-sided polygon components are composed of subunits distributed alternately, which play a crucial role in reducing the overall component number to the limitation. These findings indicate that the minimum number of components required to construct a DNA Archimedean polyhedron depends on the types of polygons involved. Additionally, our approach not only exhibits high selectivity but also offers novel insights into precise control over DNA polyhedra with specific functionalities.

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1 Introduction

The reliability and modularity of DNA make it an ideal raw material for the synthesis of functional nanostructures [1, 2]. Pre-designed DNA sequences can be folded into desired shapes, such as DNA polyhedra and two- or three-dimensional patterns [3–9], which have great potential in applications such as disease detection [10–12], drug delivery [13, 14] and biosensors [15–17]. The size and shape of these nanostructures directly impact their functionality. Therefore, there is a growing interest in developing simple strategies for designing complex DNA polyhedral structures while reducing costs. Traditionally, the principle of sequence symmetry minimization is used to avoid unintended secondary structures that may arise from mismatches between DNA strands during the pre-design process [18]. However, traditional designs often require hundreds of different individual strands of DNA for one complex structure, which can be time-consuming and costly. In contrast, a symmetric design strategy based on the principle of sequence symmetry offers inherent advantages in controlling and reducing costs by simplifying sequence design and minimizing the number of components required for DNA nanostructures. This approach has shown successful application in the design of DNA star motifs [19, 20], as well as the synthesis and investigation of one- and two-dimensional DNA patterns using only one component strand [21, 22]. Mao and his colleagues have proposed a symmetric design strategy that enables the construction of various three-dimensional DNA prisms using only two types of DNA components [23, 24]. The strategy can be extended not only to the design of simple DNA structures but also to the construction of complex DNA polyhedra, such as DNA icosahedra and Bucky balls, which are assembled from three DNA components [25]. Structures designed based on sequence symmetry offer numerous advantages, including simplified assembly processes, reduced costs and improved quality. Furthermore, the utilization of these techniques in vivo provides valuable insights into the cellular impact of each DNA strand, encompassing aspects such as biocompatibility, toxicity, immunity, and individual metabolism.

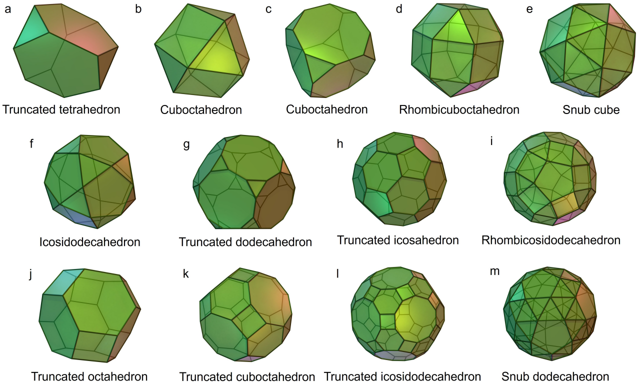

Figure 1. Perspectives diagrams of Archimedean solids

The field of DNA nanotechnology has gained significant attention due to the intriguing possibilities it offers in terms of novel DNA structures and their diverse applications. However, achieving precise control over the design of building blocks and the arrangement of these components in complex DNA polyhedra, while minimizing the number of DNA components, remains a major challenge in the realm of nanomolecular chemistry. Researchers from various disciplines, including chemistry, biology, and mathematics, have been exploring different approaches to tackle this challenge. From a synthetic perspective, chemists and biologists are working on developing strategies to achieve precise control over the design and assembly of complex DNA polyhedra. On the other hand, mathematicians have been focusing on topological approaches to minimize the number of components required for DNA polyhedra. For instance, N. Jonosk and R. Twarock proposed a method based on bead configurations to construct DNA icosahedral cages using only two strands [26, 27]. Similarly, Liu's group have constructed a family of DNA tetrahedra and analysis them by simulation [28]. Meanwhile, numerous attempts have been made to propose diverse topological strategies aiming at minimizing the number of distinct DNA single strands required for constructing various DNA polyhedral structures [29–31]. However, the practical applications of these efforts have been limited to the design of simple DNA polyhedra by changing the number of half-turns of an edge. Therefore, further extensive research is still necessary to explore and develop strategies for designing more complex DNA structures with minimal components from the aspect of sequence design. This would pave the way for breakthrough advancements in the field of DNA nanotechnology, enabling the creation of sophisticated nanostructures with enhanced functionality and diverse applications.

In this paper, we propose an approach for the design of complex DNA polyhedral structures under finite conditions. The proposed approach leverages the principle of sequence symmetry minimization and involves the development of two complementary paired subunits. These subunits serve as building blocks that can be utilized to construct various components required for the assembly of DNA polyhedra. By combining these components, a diverse range of configurations can be achieved, aiming to explore solutions that minimize the number of components involved. Our findings demonstrate that complex DNA Archimedean polyhedra can be constructed using two or more types of components, depending on the number of polygon types forming the polyhedron.

2 Complex polyhedra

Generally, Platonic polyhedra, which are considered simple polyhedra, are limited to five types. Each of them is composed solely of one type of polygon. In contrast, complex polyhedra are formed by combining two or more types of polygons. For instance, the hexahedron is comprised of six squares, while prisms and pyramids are composed of a combination of two different polygons. Figure 1 illustrates thirteen Archimedean polyhedra. For instance, a truncated tetrahedron is comprised of four triangles and four hexagons, whereas a truncated cuboctahedron contains 12 squares, 8 hexagons, and 6 octagons.

It has been demonstrated that Platonic polyhedra can be constructed using two types of components while avoiding the use of palindromic sequences. Additionally, the construction of triangular prisms and square pyramids can also be achieved using two types of components [32]. However, it is important to note that these polyhedra are considered relatively simple in their structure. In contrast, the construction of more complex polyhedra holds the potential to expand the range of potential targets for disease diagnosis and immunotherapy. Therefore, we will focus our efforts on investigating the minimum number of components needed to form an Archimedean solid, an intriguing subject we aim to demonstrate.

The regular polygons, composed of either odd or even numbers of edges, allow for the formation of different components by subunits A and B (Figure 2a). Figure 2b illustrates four distinct types of triangle components. The analysis in this paper also focuses on the varying effects that these components may have when combined to form polyhedral structures, with a particular emphasis on their role in reducing the overall component number.

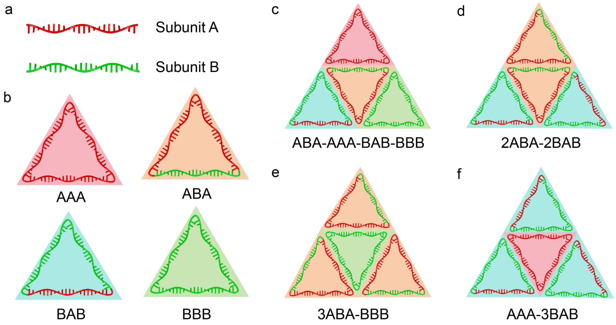

Figure 2. a) Subunits A and B; b) four different triangle components; c) a tetrahedral configuration with four components; d-f) tetrahedral configurations with two components.

3 Methods

As widely acknowledged, the majority of reported DNA polyhedra are comprised of distinct DNA single strands to ensure precise pairing. Unfortunately, this becomes time-consuming and labor-intensive for complex polyhedra, although it is inconsequential for simple ones. Hence, it is important to propose an approach that enables the design of DNA Archimedean solids with a minimal number of components.

Based on existing experimental findings, each face of a DNA polyhedron is covered by a single DNA chain, implying that every edge is wrapped around an even number of half-turns. In this context, each individual DNA chain is considered as a component, and different components are denoted by various colors. Consequently, our objective is to minimize the number of components required to construct the studied DNA polyhedron while approaching its theoretical minimum limitation.

Firstly, the target polyhedron is divided into polygons, which are further decomposed into edges based on the principle of symmetry. For instance, a tetrahedron can be divided into four triangles, and each triangle is further divided into three equal-length edges, with each edge covered by a subunit. It has been confirmed that reducing the number of subunits leads to a smaller number of component types required for constructing a polyhedron [33]. Therefore, we have designed only two complementary paired subunits, which are shown in Figure 2a. Subsequently, different types of components are formed by combining multiple subunits according to the shape of the polygons (Figure 2b). If subunit A are arranged at intervals, the components are denoted by an uppercase first letter representing the polygon followed by subscript "a" plus a number (e.g., T_{a1} and T_{a2} represent components ABA and BAB, respectively); if A and B are arranged continuously, they are represented using subscript "c" plus a number (e.g., H_c represents component AABB).

Taking the simple tetrahedron as an example, combining two subunits results in eight different components. By assembling tetrahedra with these different components, we obtain DNA tetrahedra with varying numbers of components displayed partially in Figures 2d-f. However, it was dismaying to find that even though we used the minimum number of subunits, this strategy still yields a large number of configurations. Selecting the configuration with the smallest number of components becomes challenging and computationally demanding—requiring a lot of effort.

By comparing these tetrahedral configurations, we observed that the assembly with the fewest number of components tends to be achieved through the utilization of component T_{a1} and T_{a2}. Interestingly, these statistics demonstrate a clear pattern that has been verified in convex polyhedra [33]. The question at hand is whether this tendency also holds for Archimedean polyhedra. If so, there would be no need to enumerate all possible configurations; instead, we could simply identify target configurations based on this rule and validate them accordingly. Consequently, exploring Archimedean polyhedral configurations with minimal component number becomes an uncomplicated task.

4 Results

A key characteristic of the Archimedean solids is that each face is a regular polygon, and around every vertex, the same polygons appear in the same sequence. For instance, in the depicted truncated tetrahedron, the sequence of polygons follows hexagon-hexagon-triangle. Unlike the Platonic solids which consist solely of one type of polygon, each Archimedean solid comprises two or more distinct polygons. The Archimedean polyhedra, with the exception of truncated cuboctahedron and truncated icosidodecahedron, are composed of two distinct polygons. In contrast, the truncated cuboctahedron and truncated icosidodecahedron consist of three different types of polygons.

The complementarity of subunits A and B necessitates an equal number of both. Taking the tetrahedron (Figure 2d) as an example, if two $T_{a1}s$ components are selected during combination, the remaining two can only be T_{a2} components. The difference lies in the fact that while Platonic polyhedra consist of only one type of polygon, Archimedean polyhedra are made up of multiple types of polygons, resulting in distinct situations. Some polygons are composed of odd numbers of edges (odd-sided polygon), while others consist of even numbers (even-sided polygon), thereby allowing for the formation of different components by subunits A and B.

Therefore, we need to first analyze the possibility of combining different components and the tendencies, which will help us achieve DNA Archimedean polyhedra with fewer components more efficiently. To accomplish this, the discussion should focus on three different combinations: odd-even sided polygons combination, odd-sided polygons combination, and even-sided polygons combination.

4.1 The odd-even sided polygonal components combination

The condition is satisfied by nine Archimedean polyhedra, which include truncated tetrahedron, cuboctahedron, truncated cube, rhombicuboctahedron, snub cube, icosidodecahedron, truncated dodecahedron, truncated icosahedron and rhombicosidodecahedron.

The possibilities and trends of combining odd-sided polygon components with even-sided polygon components are investigated through the utilization of a truncated tetrahedron as an illustrative example. A truncated tetrahedron consists of four triangles and four hexagons. Adhering to the rules derived from Platonic polyhedra, two alternating triangle components along with one alternating or continuous hexagon component are used to assemble a DNA truncated tetrahedron. Therefore, we can predict that the truncated tetrahedron will be assembled using three components: two triangle components ABA and BAB (T_{a1} and T_{a2}) and one hexagon component. The possible combinations are illustrated in Figure 3.

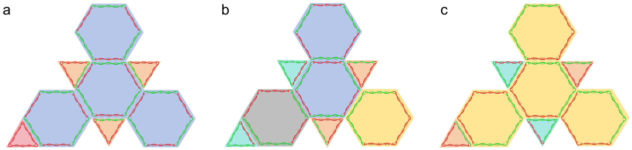

Figure 3. Possible solutions of a DNA truncated tetrahedron

The arrangement of the four H_as (ABAB) components was initially attempted, followed by an attempt to position the two $T_{a1}s$ and two $T_{a2}s$ correctly, as depicted in Figure 3a. However, despite various adjustments made, achieving the correct configuration proved unattainable without incorporating one AAA triangle component. The alternative approach involved initially placing two $T_{a1}s$ and $T_{a2}s$, followed by the introducing of H_as. However, despite our efforts, a H_c (AABB) component was necessary for a successful configuration. Consequently, the final composition (Figure 3b) comprised four distinct component types that deviated from our intended outcome. These findings imply that the desired DNA truncated tetrahedron cannot be constructed solely using H_as, $T_{a1}s$ and $T_{a2}s$

Table 1. Components of DNA complex polyhedra with odd-even sided polygons.

Polyhedra	Polygons		I	II	III	IV	V
Truncated tetrahedron	8	4 triangles 4 hexagons	$2\ T_{a1}$	$2\ T_{a2}$	$4H_c$		
Cuboctahedron	14	8 triangles 6 squares	$4\ T_{a1}$	$4\ T_{a2}$	$6S_c$		
Truncated hexahedron	14	8 triangles 6 octagons	$4\ T_{a1}$	$4\ T_{a2}$	$6O_c$		
Rhombicuboctahedron	26	8 triangles 18 squares	$4\ T_{a1}$	$4\ T_{a2}$	$18S_c$		
Snub cube	38	32 triangles 6 squares	$16\ T_{a1}$	$16\ T_{a2}$	$6S_c$		
Truncated dodecahedron	32	20 triangles 12 decagons	$10\ T_{a1}$	$10\ T_{a2}$	$12D_c$		
Truncated icosahedron	32	12 pentagons 20 hexagons	$6\ P_{a1}$	$6\ P_{a2}$	$20H_c$		
Rhomb-icosidodecahedron	62	20 triangles 30 squares	$10\ T_{a1}$	$10\ T_{a2}$	$30S_c$	$6\ P_{a1}$	$6\ P_{a2}$

in combination. Therefore, the only viable solution is to combine two $T_{a1}s$ with two $T_{a2}s$ alongside four H_cs in a logical manner resulting in the final configuration displayed in Figure 3c.

The results depicted in Figure 3 illustrate the strategy for achieving the DNA polyhedron with minimal components through coordinated assembly of odd-even sided polygonal components. Additionally, they indicate that when combining odd-even sided polygonal components, the subunits A or B within even-sided polygonal components tend to adopt a contiguous arrangement.

Subsequently, we applied this rule to construct the remaining eight polyhedra, resulting in the successful attainment of optimal target structures as outlined in Table 1. This unequivocally demonstrates that our findings possess a highly influential capacity for guiding the design of DNA Archimedean polyhedra with minimal component number. Obviously, for an odd-sided polygons, a minimum of two distinct components is required, while for an even-sided polygons, at least one distinct component is necessary. If the target polyhedron adheres to this principle, the optimal structure obtained will inevitably possess the fewest possible components.

4.2 The odd-sided polygonal components combination

The snub dodecahedron is comprised of triangles and pentagons, thus necessitating an examination of the combination rules governing these components through local analysis. As depicted in Figure 4a and b, we observe numerous possibilities when attempting to position five triangle components around a P_{c1} (AAABB) or P_{a2} (BABAB) component; however, the final outcome depends not only on P_{c1} or P_{a2} but also on the configuration of other surrounding pentagon components. Similar results emerge when trying to position three pentagon components adjacent to a T_{a1} or T_{a2} component (Figure 4c and d). Evidently, for polyhedra comprised of odd-sided sided polygons like these, local exploration proves unsuitable and instead necessitates adopting a strategy involving global attempts.

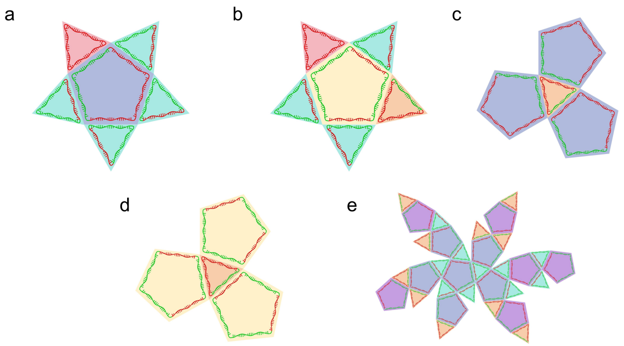

Figure 4. Possibilities of odd-sided polygonal components combination

Therefore, we systematically investigated various configurations and ultimately identified the snub dodecahedral arrangement comprising ten $T_{a1}s$, ten $T_{a2}s$, six $P_{c1}s$, and six $P_{c2}s$ as illustrated in Figure 4e. The minimum number of components required for constructing a DNA snub dodecahedron is four, as outlined in Table 2. Although the local exploration reveals numerous possibilities, we observed a contiguous distribution of subunits A or B of these odd-sided polygons when applied to the target polyhedra. This intriguing phenomenon demonstrates that the components utilized for assembling polyhedra with minimal component numbers exhibit a similar pattern as previously concluded.

Table 2. Components of DNA complex polyhedra with odd-sided polygons.

Polyhedra	Polygons		I	II	III	IV
Icosi-dodecahedron	32	20 triangles 12pentagons	10 T_{a1}	10 T_{a2}	6 P_{c1}	6 P_{c2}
Snub dodecahedron	92	80 triangles 12 pentagons	40 T_{a1}	40 T_{a2}	6 P_{c1}	6 P_{c2}

4.3 The even-sided polygonal components combination

The truncated octahedron, truncated cuboctahedron, and truncated icosidodecahedron are composed exclusively of even-sided polygons. Specifically, a truncated octahedron comprises 6 squares and 8 hexagons, a truncated cuboctahedron consists of 12 squares, 8 hexagons, and 6 octagons, while a truncated icosidodecahedron is composed of precisely 30 squares, 20 hexagons, and 12 decagons. Given the incorporation of both squares and hexagons in these polyhedra structures, we aim to elucidate the various possible combinations between these two polygonal shapes.

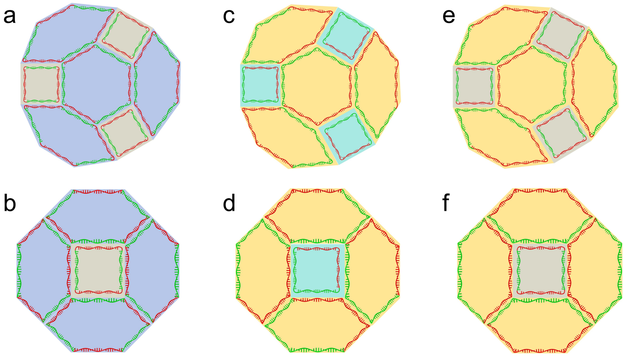

Figure 5. Possibilities of even-sided polygonal components combination

In Figure 5a, one component H_a is centrally positioned, while the remaining three identical Has are arranged around it to maintain an unchanged component count. As a result, only three $S_a s$ (ABAB) can be accommodated since $S_c s$ (AABB) fail to meet the specified requirements. Conversely, by adhering to the principle of complementary base pairing

Table 3. Components of DNA complex polyhedra with even-sided polygons.

Polyhedra	Polygons		I	II	III
Truncated octahedron	14	6 squares 8 hexagons	6 S_c 6 S_a 6 S_a	8 H_c 8 H_c 8 H_a	
Truncated cuboctahedron	26	12 squares 8 hexagons 6 octagons	12 S_c 6 S_a	8 H_c 8 H_a	6 O_c 6 O_a
Truncated icosidodecahedron	62	30 squares 20 hexagons 12 decagons	30 S_c 30 S_a	20 H_c 20 H_a	12 D_c 12 D_a

(Figure 5b), four $H_a s$ can also be arranged adjacent to a component S_a. The results indicate that both $S_a s$ and $S_c s$ fulfill our requirements when a single H_c is positioned in the center using the same approach, as illustrated in figures 5c and e. When tested in reverse, these results remain consistent, as depicted in figures 5d and f. However, it is not feasible to position four $H_a s$ around the central S_c.

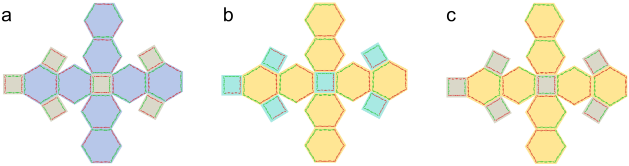

Figure 6. Three possible configurations of a truncated octahedron with three components

The results presented herein demonstrate that in order to achieve DNA polyhedra with the minimum number of components using even-sided polygon components, the arrangement of subunits A and B can be either alternating or contiguous, depending on the specific design schemes. Importantly, it should be noted that this arrangement is also adopted by other components when subunits A and B are arranged within one component, thereby facilitating the construction of DNA polyhedra with a reduced number of components.

Subsequently, we utilized this rule to construct a truncated octahedron and obtained three configurations comprising two distinct components: six $S_a s$ and eight $H_a s$ (Figure 6a), six $S_c s$ and eight $H_c s$ (Figure 6b and 6c). By avoiding exhaustive enumeration, we can identify two DNA truncated

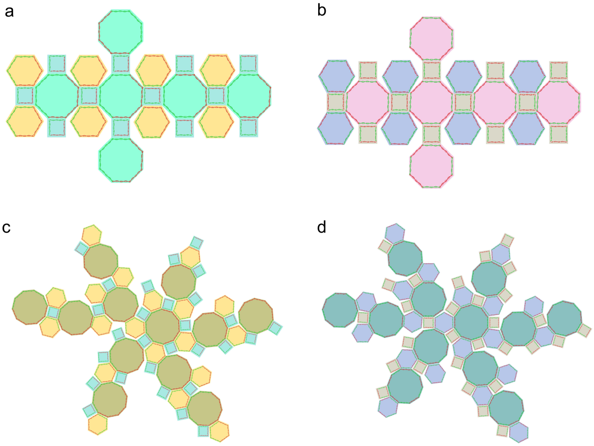

Figure 7. a,b) Two possibe configurations of a truncated cuboctahedron with three components; c,d) Two possibe configurations of a truncated icosidodecahedron with three components

cuboctahedra configurations depicted in Figure 7a and as well as two DNA truncated icosodecahedra configurations illustrated in Figure 7c and d. The specific details regarding their constituent components are listed in Table 3.

5 Discussion

By investigating the potential configurations of various DNA Archimedean polyhedra under the limitation of using only two subunits, we construct a series of synthetic candidate structures with minimal component counts. Additionally, we analyze the impact of different components when combined to form polyhedral structures with the fewest number of components. Distinct trends are observed in the combinations of odd-sided polygon components even-sided polygon components. In the combination of odd-even polygons, Figure 3 illustrates the resulting configurations, while Table 1 provides detailed information indicating that even-sided polygon components tend to reduce their symmetry to form polyhedra with minimal component number. For instance, a truncated tetrahedron with only three components requires four H_cs components; evidently, H_c less symmetrical than H_a. Similar conclusions can be drawn for all polyhedra composed of both odd and even polygons.

In contrast, the combination of different even-sided polygonal components does not necessarily require a reduction of symmetry in the arrangement of subunits. While reduced symmetry is not essential for polyhedra composed of even-sided polygons, lower symmetry components can also contribute to the formation of DNA polyhedra with fewer components. Polyhedra with a smaller number of components require these components to adopt lower levels of symmetry. Conversely, as the number of components increases, it becomes more advantageous for them to possess lower levels of symmetry, thereby facilitating the generation of DNA polyhedra. This observation may elucidate why most DNA polyhedra have been designed based on minimizing sequence symmetry.

Based on the aforementioned rules, a series of Archimedean polyhedra with the minimum number of components are constructed. From an academic standpoint, what is particularly intriguing is that these rules not only apply to simple Platonic polyhedra but also extend to complex Archimedean polyhedra. Consequently, a more generalized conclusion can be drawn as follows: for a given polyhedron P composed of identical or different polygons, the minimum number of components is 2m + n, if P consists of m types of odd-sided polygons and n types of even-sided polygons. The minimum number of components is two if P comprises identical odd-sided polygons. A classic example would be a DNA tetrahedron consisting of two $T_{a1}s$ and two $T_{a2}s$. On the other hand, if P consists solely of identical even-sided polygons, reduces to one; for instance, in the case of a DNA cube composed entirely by six S_as or six S_cs. Similarly, due to its composition involving three distinct types of even-sided polygons, a truncated icosidodecahedron can be assembled using three kinds of components.

The DNA polyhedral configurations obtained through our strategy are not only unique but also provide valuable insights into their precisely control and specific functions. With the advancement of DNA nanostructure synthesis techniques, we have effectively addressed the potential impact on yield, stability, size, and shape arising from the utilization of repeated two subunits in our proposed approach. Also, our highly selective strategy can enable the synthesis of these structures with precision, which in turn facilitates exploration of the cellular impact and metabolic processes associated with each DNA strand.

6 Conclusion

In this study, two subunits were designed and utilized for the construction of a series of odd-sided polygonal and even-sided polygonal components. Specifically, in the formation of DNA polyhedra with the minimum component number, the subunits within even-sided polygonal components tend to be distributed contiguously or alternately, while those within odd-sided polygonal components tend to be alternately distributed. These distinct components are subsequently combined to form various Archimedean polyhedra based on their inherent geometries. Furthermore, we elucidate a general rule for designing DNA polyhedra with minimal component numbers: given a polyhedron P composed of m types of odd-sided polygons and n types of even-sided polygons, its minimum component number is 2m + n. Meanwhile, our strategy exhibits excellent selectivity, enhanced control capabilities, and ease-of-use; thus, providing valuable insights for design and chemical synthesis.

The research on component number reveals that although most of these aesthetic and extremely complex architectures can be synthesized using a few components. This implies that they will serve as novel candidates for chemical synthesis and future applications, especially in the field of complex DNA cages. However, the mechanism governing the generation of DNA polyhedra with minimal components remains elusive, and further mathematical proofs and dynamic analyses are still necessary.

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