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Original article

The uniqueness of perfect star packings and the existence of pseudo-matchings in (2,6)-fullerene graphs

Meysam Taheri-Dehkordi[1,a]

[1]University of Applied Science and Technology, Tehran, Iran

[a]m.taheri@uast.ac.ir

Corresponding author: Meysam Taheri-Dehkordi, m.taheri@uast.ac.ir

ABSTRACT A perfect star packing can be described as a spanning subgraph whose connected components are isomorphic to the star graph $K_{1,3}$. A perfect pseudo-matching is a spanning subgraph in which every component is isomorphic to either K_2 or $K_{1,3}$. The study of packing problems on fullerene graphs is of particular interest due to their potential relevance in describing local bonding arrangements in carbon nanostructures. In this paper, we study the uniqueness of perfect star packing, and the existence of pseudo-matchings in $(2,6)$-fullerene graphs. Moreover, we show that the perfect star packing in these graphs is unique. Furthermore, we introduced some perfect pseudo-matchings in $(2,6)$-fullerene graphs.

KEYWORDS $(2,6)$-fullerene graphs; perfect star packing; perfect pseudo-matching.

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1. Introduction

Fullerenes are carbon atom-based polyhedral molecules. They come in various sizes and forms. Fullerene graphs serve as a crucial mathematical structure for modeling carbon-based nanosystems, with vertices depicting carbon atoms and edges representing covalent bonds [1]. The study of structural properties of fullerene graphs has long been motivated by their close relationship with real carbon cages and nanotube-related nanostructures [2]. Also, theoretical research on fullerenes in graph theory, in parallel with experimental experiments, has led to the identification of structural properties of stable fullerenes at macroscopic quantities. These theoretical researches have led to the investigation and prediction of the potential stability of these molecules.

One of the most interesting patterns in fullerenes is the one that allows for a resonance structure. But such patterns should not overlap, so they are modeled by packings in the corresponding graphs. A $(k,6)$-fullerene graph is defined as a planar cubic graph in which every face is bounded by either k-cycles or 6-cycles. Došlić [3] established that such graphs exist only for $k = 2,3,4$ and, 5. Applying Euler's formula, one can deduce that the number of k-length faces in $(k,6)$-fullerenes graphs for $k = 2,3,4$ and 5 equals $3,4,6$ and 12, respectively. For a graph G, a matching M is defined as a set of edges of G in which no two edges share a common vertex M. A matching is perfect if every vertex of G is incident to exactly one edge from M. In addition to mathematics, perfect matchings have also received much attention in chemistry and are known as the Kekulé structures.The number of Kekulé structures in a benzenoid hydrocarbon is intricately connected to the compound's stability. In a graph G, a perfect star packing can be described as a spanning subgraph whose connected components are isomorphic to the star graph $K_{1,3}$. Similarly, a perfect pseudo-matching is a spanning subgraph where each component is isomorphic to either K_2 or $K_{1,3}$. When all components are edges K_2 the structure forms a perfect matching, and, when all are stars $K_{1,3}$ it becomes a perfect star packing. While a pseudo-matching matching containing both types of components is called mixed pseudo-matching. Researching packing problems in fullerene graphs is intriguing because of their possible significance to local bonding configurations in nanoscale carbon structures [4,5].

Specifically, the aim of this research is to investigate the conditions under which the addition of bulky groups leads to maximum efficiency and how many bulky groups (i.e., addition to one atom prohibits addition to other atoms) can be added so that the remaining part of the molecule still has a resonance structure. The concept of packing is very useful for modeling such a situation. Understanding the uniqueness and existence of perfect star packings and pseudo-matchings in (2,6)-fullerene graphs provides insight into the structural rigidity, stability, and possible functional patterns of such nanoscale systems. Motivated by these connections, the present paper investigates the uniqueness of perfect star packings and the existence of perfect pseudo-matchings in (2,6)-fullerene graphs, highlighting their potential importance for nanoscale structural modeling.

Extensive research has been conducted on fullerene graphs for $k = 3, 4$, and, 5. However, comparatively fewer studies have focused on $(2, 6)$-fullerene graphs. In [4, 6, 7], the authors have obtained results about perfect star packings of $(k, 6)$-fullerene graphs for $k = 3, 4$ and, 5. Taheri-Dehkordi and Fath-Tabar [8], examined nice pairs of pentagons in chamfered fullerenes. Some properties of these graphs have been examined in [9–14]. Reference [15] provides the computation of the number of perfect star packings and pseudo-matchings in some types of fullerene graphs. Yang et al. [16], investigated the structure of $(2, 6)$-fullerene graphs. In a recent paper [17], the existence of perfect star packing in $(2, 6)$-fullerene graphs was investigated. In this paper, we determine the number of perfect star packings and mixed pseudo-matchings in $(2, 6)$-fullerene graphs by considering their structural properties and the arrangements perfect star packing of these graphs.

2. Definitions and auxiliary results

This section states the important and used definitions and preliminary results. A $(2, 6)$-fullerene graph can be characterized as a cubic planar graph in which all faces lengths are either 2 or 6. By Euler's formula, these graphs contain exactly three 2-length faces. The structure of some $(2, 6)$-fullerene graphs is stated in [16]. The authors proved that there are $(2, 6)$-fullerene graphs with f_G hexagonal faces, so that f_G depends on a parameter such as s. In a $(2, 6)$-fullerene graph G, a **fragment** H refers to a subgraph that consists of a cycle and the region inside it, such that all faces contained in this interior are also faces of G [16]. In this study, four types of $(2, 6)$-fullerene graphs with the following structure were introduced.

$(2, 6)$-Fullerene graphs of type 1: These graphs consist of a fragment G_s as shown in Fig. 1, which consists of s hexagonal layers.

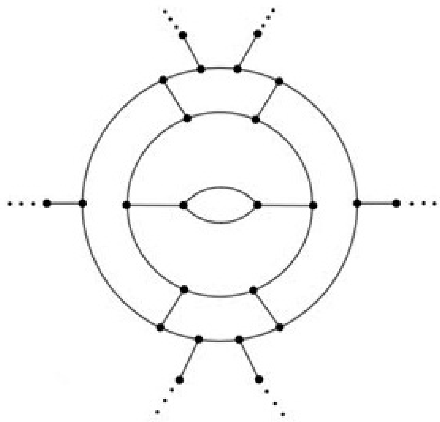

FIG. 1. The fragment G_s in $(2, 6)$-Fullerene graphs of type 1

$(2, 6)$-Fullerene graphs of type 2: These graphs consist of a fragment C_s as shown in Fig. 2, which consists of s hexagonal layers.

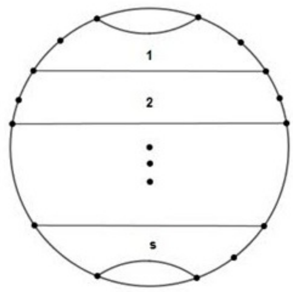

FIG. 2. The fragment C_s in $(2, 6)$-Fullerene graphs of type 2

$(2, 6)$-Fullerene graphs of type 3: These graphs consist of an initial fragment as shown in Fig. 3.

$(2, 6)$-Fullerene graphs of type 4: These graphs consist of a fragment F_6 as shown in Fig. 4.

In [17], based on this structure, the existence of perfect star packing in these graphs is investigated. We summarize these results below.

Proposition 2.1 ([17]). *If G be a $(2, 6)$-fullerene graphs of type 1 with s hexagonal layers. Then,*

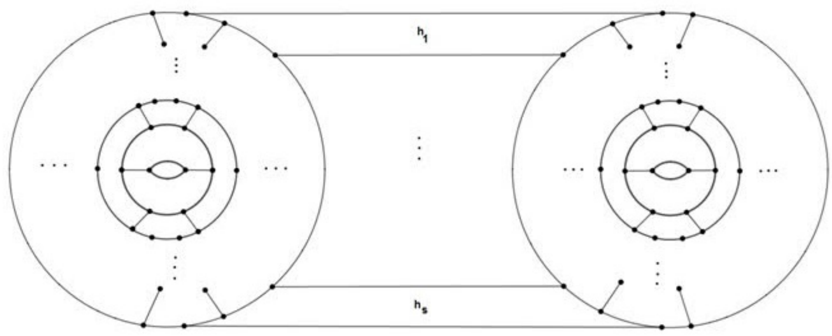

FIG. 3. The initial fragment in $(2,6)$-fullerene graph of type 3

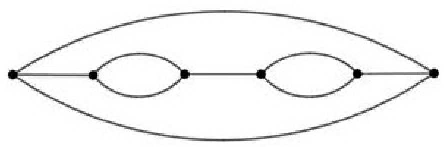

FIG. 4. The fragment F_6 in $(2,6)$-fullerene graph of type 4

(1) *If s is odd, then G has a perfect star packing.*
(2) *If s is even, then G does not admit a perfect star packing.*

Proposition 2.2 ([17]). *If G be a $(2,6)$-fullerene graphs of type 2 with s hexagonal faces in the first layer. Then,*

(1) *If s is odd, then G has a perfect star packing.*
(2) *If s is even, then G does not admit a perfect star packing.*

Proposition 2.3 ([17]). *Let G be a $(2,6)$-fullerene graphs of type 3 with s hexagonal layers in their fragments. Then,*

(1) *If s is odd, then G admit a perfect star packing.*
(2) *If s is even, then G does not admit a perfect star packing.*

Proposition 2.4 ([17]). *Let G be a $(2,6)$-fullerene graphs of type 4. Then, G does not have a perfect star packing.*

3. Number of perfect star packing in $(2,6)$-fullerene graphs

In this section, according to the structure of perfect star packings of (2,6)-fullerene graphs, introduced in [17], we calculate the number of these packings and mixed perfect pseudo-matchings in four types of these graphs. Following the notation introduced in [15], $PSP(G)$ denotes the number of perfect star packings in the graph G.

In [17], a method for the perfect star packing in (2,6)-fullerene graphs of type 1 was presented. This packing configuration is denoted by, P_1. We show that in this type of fullerene graphs, there is no other method for packing, and also, only one packing configuration can be considered in this method. In other words, this packing is unique.

Theorem 3.1. *Let G be a $(2,6)$-fullerene of type 1. Then, $PSP\,(G) = 0$ if s is even and, $PSP\,(G) = 1$ if s is odd.*

Proof. According to Proposition 2.1, if s is even, G does not admit a perfect star packing and therefore, $PSP\,(G) = 0$. Assume that s is odd. First, we consider the innermost layer. For packing this layer, vertices v_0 and $v_0{}'$ designated as the central vertices of the star structure (see Fig. 5). Also, in the last layer to cover vertices w_1, w_2, w_3, and w_4, vertices $w_1{}'$, $w_2{}'$, $w_3{}'$, and $w_4{}'$ must be the central vertex of the star, respectively.

In the second layer, to cover the vertex u_0, either u_0 itself must be the star's central vertex or $u_0{}^{'}$, (Fig. 6). If u_0 is the star's central vertex, then we obtain the same packing as P_1. So, Assume that $u_0{}^{'}$ is the central vertex of the star.

To cover u_1, the vertex $u_1{}'$ must necessarily be the central vertex of the star. To cover the vertex u_2, we consider the following two cases.

(1) $u_2{}'$ is a central vertex. In this case, to cover vertex u_3, vertex $u_3{}'$ must be the central vertex of the star. Also, to cover vertex u_4, vertex $u_4{}'$ must be the central vertex of the star. Under these conditions, u_5 is not covered.
(2) u_3 is a central vertex. In this case, to cover vertex u_5, vertex $u_5{}'$ must be the central vertex of the star. Likewise, to cover u_6, vertex u_7 must be the central vertex, and to cover u_8, vertex $u_8{}'$ must be the central vertex of the star (Fig. 7). In this case, $u_4{}'$ is not covered.

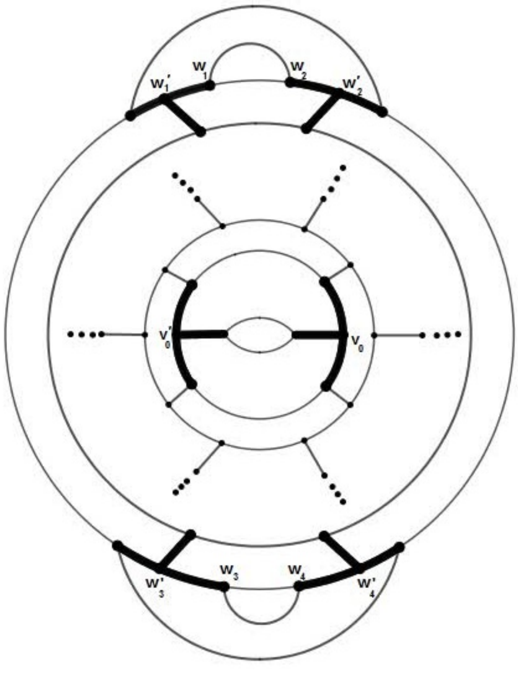

FIG. 5. Packaging in the first and last layers

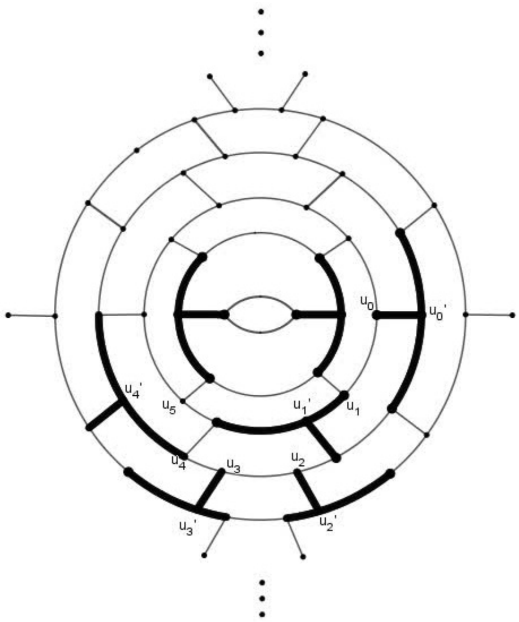

FIG. 6. Packing in the second layer

Hence, it is impossible to obtain a perfect star packing in either case, implying that ${u_0}'$ cannot be the central vertex and u_0 must be a central vertex of the star.

From the above discussion, conclude that we should have the same P_1 packing method in the second and third layers. On the other hand, subsequent layers must also be packing in pairs. Therefore, P_1 is the only packing method. Now, we need to check if there is another way to packing with this method. As mentioned, there is only one state in the first layer. An even number of layers remain, which are packed in pairs. The only way to increase the number of packing states in a pair of layers, is to rotate the stars. We consider the k-th and $(k+1)$-th arbitrary layers, where k is an even number. There are $4k+2$ and $4k+6$ vertices in these two layers, respectively, and there are $2k+2$ star graphs in these two layers. The packing of these two layers is shown in Fig. 8.

In the neighborhood of each of the stars S_1, S_2, S_3 and S_4, there must be a star with a central vertex in the k-th layer. (stars ${S_1}'$, ${S_2}'$, ${S_3}'$ and ${S_4}'$ in Fig. 9).

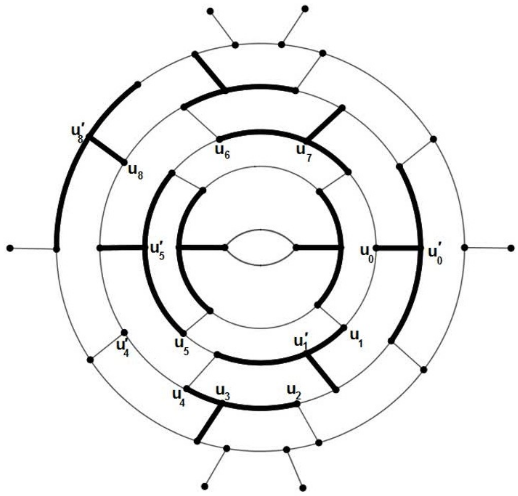

FIG. 7. Covering the vertex u_2

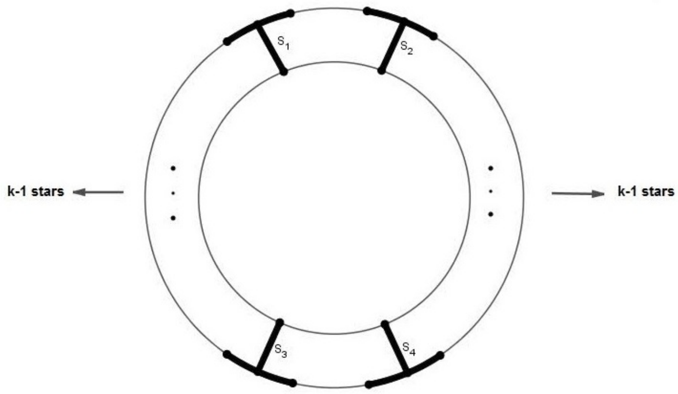

FIG. 8. Packing in two arbitrary layers

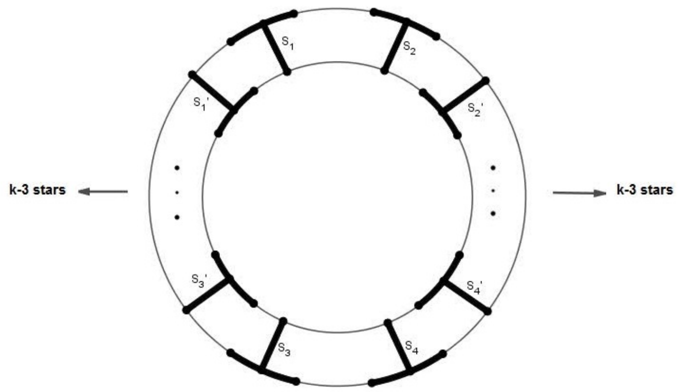

FIG. 9. Packing in two arbitrary layers

Also, adjacent to each of these star graphs, there must be a star graph with a central vertex in the $k + 1$-th layer. Continuing this process, we will again arrive at the packing P_1. □

In [17], one technique to obtain a perfect star packing in (2,6)-fullerene graphs of type 2 and type 3 was presented. We call these packings P_2 and P_3, respectively. In the following theorems, we show that in these types of fullerene graphs, there is no other method for packing, and also, only one packing configuration can be considered in two methods. In other words, these packings are unique.

Theorem 3.2. *Let G be a $(2, 6)$-fullerene of type 2. Then, $PSP\,(G) = 0$ if s is even, and $PSP\,(G) = 1$ if s is odd.*

Proof. According to Proposition 2.2, if s is even, G does not have a perfect star packing and therefore, $PSP\,(G) = 0$. Now, assume that s is odd. If we want to have a packing other than P_2, the edges e_1, e_2, e_3 and e_4 should be considered as star edges (see Fig. 10).

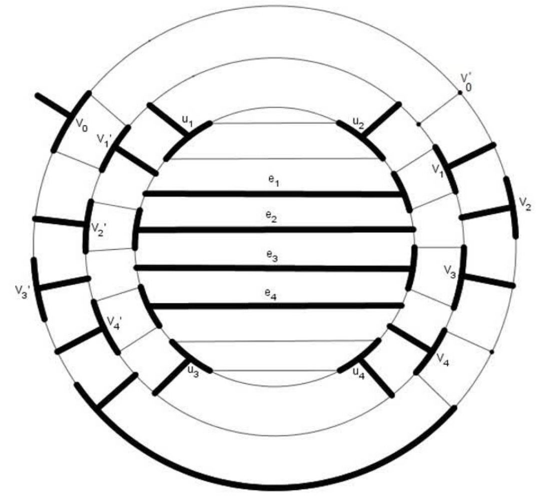

FIG. 10. A packing in G

It is necessary that u_1, u_2, u_3 and u_4 be the central vertex of the star. Also, vertices v_1, v_2, v_3, v_4 v_1', v_2', v_3' and v_4' are also the central vertices of the star. To cover the vertex v_0, this vertex itself must be the central vertex, and in this case, vertex $v_0{}'$ is not covered. Therefore, the only packing method in this type of graph is the P_2 packing. Now, we prove that there is only one state for this type of packing, and we conclude that $PSP\,(G) = 1$. In the first two layers, due to the structure of 2-length cycles, there is only one state for packing. Now, we consider the third and fourth layers. In the packing P_2, the vertex v_1 is the star's central vertex (Fig. 11), and the vertex v_1 is also covered.

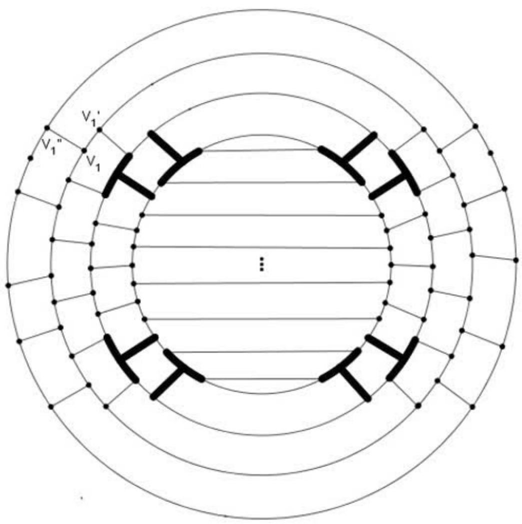

FIG. 11. Packing of vertices

If we want to consider vertex $v_1{}''$ as the central vertex of the star, then $v_1{}'$ is not covered in any other way, so changing the packing in this layer is also not possible. In other layers, similar to what was stated in Theorem 3.1, the rotation of stars is not possible, and therefore, the statement is proven. □

Theorem 3.3. *Let G be a $(2,6)$-fullerene of type 3. Then, $PSP(G) = 0$ if s is even and, $PSP(G) = 1$ if s is odd.*

Proof. According to Proposition 2.3, if s is even, G does not admit a perfect star packing and therefore, $PSP(G) = 0$. Now, assume that s is odd. In $(2,6)$-fullerene graphs of type 3, the packing of the initial fragment is done according to the packing of $(2,6)$-fullerene graphs of type 1. Therefore, this type of packing is unique. In the last layer, we also have a unique packing. What remains are the remaining layers, the number of which is even. In these layers, as in the proof of Theorem 3.1, rotation of stars is not possible, and therefore, $PSP(G) = 1$. □

It is proved in [17] that $(2,6)$-fullerenes of type 4 do not admit a perfect star packing. Considering this, the following theorem can thus be deduced.

Theorem 3.4. *Let G be a $(2,6)$-fullerene of type 4. Then, $PSP(G) = 0$.*

4. Perfect pseudo-matchings in $(2,6)$-fullerene graphs

In the present section, we examine the mixed perfect packings, commonly referred to as pseudo-matchings. In a graph G, a perfect pseudo-matching is a spanning subgraph whose connected component is either a K_2 or a $K_{1,3}$.

Theorem 4.1. *Every $(2,6)$-fullerene of type 1 with an odd number of hexagonal layers has a perfect matching.*

Proof. According to Theorem 3.1, $(2,6)$-fullerene graphs with an odd number of layers admits a unique perfect star packing consisting of $\frac{n}{4}$ star graphs $K_{1,3}$. (n is the number of vertices of graph). Using this packing, we construct a matching M for this type of graphs. Let G be a $(2,6)$-fullerene of type 1 with an odd number of hexagonal layers. In the first layer, we consider the matching edges as shown in Fig. 12 (dashed lines).

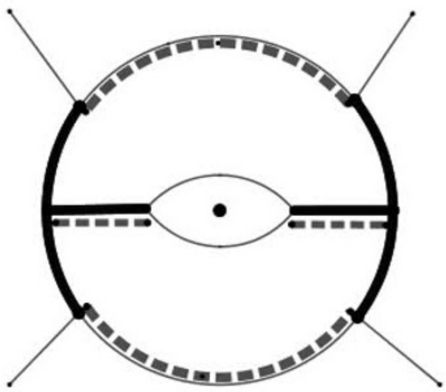

FIG. 12. Matching in the first layer

In other layers, at one pole, for two pairs of layers G, we consider the edges of M as shown in Fig. 13(a) (dashed lines). At the other pole, the edges of M are considered as shown in Fig.13(b).

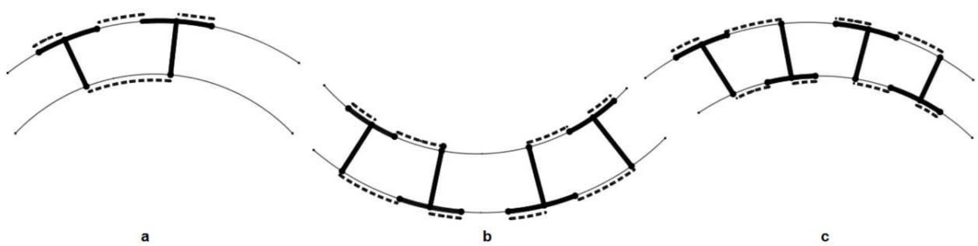

FIG. 13. Matching at two poles and two pairs of layers

In other parts, we consider the edges of M in each pair of layers as shown in Fig. 13(c) (dashed lines). Therefore, all vertices are covered by K_2 components, and thus, a perfect matching for G is obtained. □

Theorem 4.2. *Let G be a $(2,6)$-fullerene of type 1 with an odd number of hexagonal layers. Then, G contains a mixed perfect pseudo-matching comprising at least two star components.*

Proof. It is established that G admits a perfect star packing. To prove the claim, it is necessary to demonstrate that G contains two copies of $K_{1,3}$ whose union forms a nice subgraph of G. For this purpose, we consider the process of forming the graph matching in Theorem 4.1. In this matching, we consider each pair of $K_{1,3}$ star graphs. Suppose that k_1 and k_2 are two adjacent star graphs. For other star graphs in the perfect star packing, we follow the process of constructing the matching. By doing this, $G - \{k_1, k_2\}$ has a perfect matching and therefore, $k_1 \cup k_2$ is a nice subgraph of G. □

By performing the method mentioned in the proof of Theorem 4.2 for each pair of stars, the following corollary can be obtained.

Corollary 4.3. *Every* $(2, 6)$*-fullerene of type 1 with an odd number of hexagonal layers contains a mixed perfect pseudo-matching with at least two star components.*

Table 1 presents the number of K_2 and $K_{1,3}$ components in a mixed perfect pseudo-matching in $(2, 6)$-fullerenes of type 1 with an odd number of hexagonal layers.

TABLE 1. Number of components in mixed perfect pseudo-matching

Number of $K_{1,3}$ components	Number of K_2 components
$\frac{n}{4}-2$	4
$\frac{n}{4}-4$	8
$\frac{n}{4}-6$	12
$\frac{n}{4}-8$	16
...	...

Considering the process of defining perfect star packing in $(2, 6)$-fullerene graphs of types 2 and 3 and, similar to what was stated in the proof of Theorems 4.1 and 4.2, the following Theorems can be stated.

Theorem 4.4. *Let* G *be a* $(2, 6)$*-fullerene of type 2 or 3 with an odd number of hexagonal layers. Then,* G *has a perfect matching.*

Theorem 4.5. *Let* G *be a* $(2, 6)$*-fullerene of type 2 or 3 with an odd number of hexagonal layers. Then,* G *contains a perfect pseudo-matching with at least two star components.*

5. Conclusion

In this study, our results demonstrated that for types 1, 2, and 3, perfect star packings are unique. Moreover, we established the existence of perfect pseudo-matchings containing both star and matching components for the same classes of graphs. These findings contribute to a deeper understanding of the combinatorial and structural properties of fullerene graphs and may serve as a foundation for further investigations into their packing and matching configurations. The results obtained from a nano-systems science point of view describe local structural motives in carbon nanostructures based on the $(2, 6)$-fullerenes. The uniqueness of perfect star packings shows that there is only one predominant type of local coordination - something that could be interpreted as an indication of structural stability and a reduced configurational ambiguity at the nanoscale. Therefore, the outcome of the present work can be of benefit to a wider understanding of structure-property relationships in nanoscale systems, where graph theory plays a very important role in connecting mathematics with chemistry.

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Information about the authors:

Meysam Taheri-Dehkordi – University of Applied Science and Technology, Tehran, Iran; ORCID 0000-0002-6085-2622; m.taheri@uast.ac.ir

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