



Induced H -packing k -partition problem in certain carbon based nanostructures

Santiago Theresal¹ · Antony Xavier¹ · S. Maria Jesu Raja²

Received: 28 July 2020 / Accepted: 18 February 2021

© The Author(s), under exclusive licence to Springer Nature Switzerland AG 2021

Abstract

Nanotechnology has gained recently much attention in research to develop new carbon based materials with unique properties. It generates many new materials and devices with a wide range of applications in medicine, electronics, and computer. Carbon nanotubes ($CNTs$) are one of the most promising resources in the field of nanotechnology. Mathematically, assembling in predictable arrays is equivalent to packing in graphs. An H -packing of a graph G is the set of vertex disjoint subgraphs of G , each of which is isomorphic to a fixed graph H . In this paper we determine perfect and almost perfect H -packing and an induced H -packing k -partition number for Armchair carbon nanotube $ACNT[n, m]$, Zigzag carbon nanotube $ZCNT[n, m]$, Zigzag polyhex carbon nanotube $TUHC_6[2m, n]$, Boron triangular carbon nanotubes $BNT_t[n, m]$, $TUC_4C_8(R)$, $TUC_4C_8(S)$, $HAC_5C_6C_7[n, m]$ and $HAC_5C_7[n, m]$ with H isomorphic to P_3 . Further we investigate C_4 -packing for $TUC_4C_8(R)$.

Keywords P_3 -packing · C_4 -packing · Perfect P_3 -packing · Perfect C_4 -packing · Almost Perfect P_3 -packing · Induced P_3 -packing k -partition · Armchair carbon nanotube $ACNT[n, m]$ · Zigzag carbon nanotube $ZCNT[n, m]$ · Zigzag polyhex carbon nanotube $TUHC_6[2m, n]$ · Boron triangular carbon nanotubes $BNT_t[n, m]$ · $TUC_4C_8(R)$ · $TUC_4C_8(S)$ · $HAC_5C_6C_7[n, m]$ · $HAC_5C_7[n, m]$

1 Introduction

Carbon Nanotube Science is the most concise, accessible book for the field, presenting the basic knowledge graduates and researchers need to know [10]. Carbon nanotubes are large macromolecules that are unique for their size, shape, and remarkable physical

✉ Santiago Theresal
santhia.teresa@gmail.com

¹ Department of Mathematics, Loyola College, (Affiliated to University of Madras), Chennai 600 034, India

² School of Basic Sciences, VISTAS, Chennai 600 117, India

properties. They are molecular-scale tubes of graphitic carbon with outstanding properties. Carbon nanotubes are one of the most commonly mentioned building blocks of nanotechnology. They show remarkable mechanical properties. Experimental studies have shown that they belong to the stiffest and elastic known materials [14,27].

Chemical graph theory is a subdivision of mathematical chemistry in which we apply tools of graph theory to represent the chemical phenomenon mathematically. This theory plays a prominent role in the fields of chemical sciences. A chemical graph is a simple finite graph in which vertices denote the atoms and edges denote the chemical bonds in underlying chemical structure [18].

Carbon Nanostructures have attained significant attention due to their potential use in many applications including biosensors, nano-electronic devices, chemical probes, gas sensors and energy storage [14]. Nanotube structures have many applications in the general field of nanotechnology, which is a relatively recent field with much potential, as well as some significant liabilities. Structures realized by arrangements of regular hexagons in the plane are of interest in the chemistry of benzenoid hydrocarbons, where perfect matchings correspond to Kekulé structures which feature in the calculation of molecular energies associated with benzenoid hydrocarbon molecules [8]. Various surface nanotemplates that are naturally or artificially designed at the nanometre scale have been used to form periodic nanostructure arrays [20].

Mathematically, assembling in predictable patterns is equivalent to packing in graphs. Packing in graphs is an effective tool as it has lots of applications in applied sciences. Packing is one of the most extensively studied problem in computer science, mainly due to its combinatorial aspects and algorithmic implementations. Packing theory have useful applications to code optimization, clustering, component placing, wireless sensor tracking, wiring-board design and many others [4,12,13]. The packing problem is also used in dynamic channel assignment for cellular radio communication systems [16]. In addition to this, academic researchers work to create tiny circuits using nodes that automatically arrange themselves into useful patterns [9].

An H -packing in a graph $G = (V, E)$ is a set of vertex disjoint induced subgraphs of G , each of which is isomorphic to a fixed graph H [23]. A cycle in graph theory is a closed trail whose origin and internal vertices are distinct [2]. The maximum number of vertex disjoint copies of H in G is called the packing number and is denoted by $\lambda(G, H)$. A perfect H -packing in a graph G is a set of H -subgraphs of G such that every vertex in G is incident with one H -subgraph in this set. An almost perfect H -packing in a graph G is a set of H -subgraphs of G such that at most $|V(H)| - 1$ number of vertices are not incident on any H -subgraph in G [23]. The P_3 -packing concepts have some applications in chemistry for representing chemical compounds or to problems of pattern recognition and image processing, some of which involve the use of hierarchical data structures of nanotubes [26]. An H -packing is of practical interest in the areas of scheduling [1], wireless sensor tracking [3], wiring-board design, code optimization [11] and many others. Packing lines in a hypercube has been studied in [7]. H -packing is determined for honeycomb [25] and hexagonal network [21]. An induced H -packing k -partition problem was studied for interconnection networks [23]. An induced P_3 -packing k -partition was studied for butterfly networks, honeycomb networks and Circum Pyrene [30]. Xavier et al [28] proved an induced P_3 -packing k -partition number for Enhanced hypercubes, Augmented cubes and

Crossed cubes with $H \simeq P_3$ and C_4 . An induced H -packing k -partition is determined for V -Phenylenic nanotube, H -Naphthalenic nanotube, H -Anthracenic nanotube, H -Tetracenic nanotube, $CNC_3[n]$ Nanocone and Circum tetracene with $H \simeq P_3$ [29].

Partitioning a network with respect to vertices, edges or subgraphs is a significant aspect in enlarging resource utilization of parallel machines. Partitioning large networks is often important for complexity reduction or parallelization. For instance, in telecommunication networks, same frequency can be assigned to different subnetworks if the frequencies do not interfere with each other. Thus the study of partitioning a H -packing such that no two members in the same partition interfere, becomes meaningful [23]. But partitioning nanotubes with respect to vertices, edges and subgraph is a new concept that deal with representing chemical compounds and in the use of hierarchical data structures in Armchair carbon nanotube $ACNT[n, m]$, Zig-Zag carbon nanotube $ZCNT[n, m]$, Zig-Zag polyhex carbon nanotube $TUHC_6[2m, n]$, Boron triangular carbon nanotubes $BNT_t[n, m]$, $TUC_4C_8(R)$, $TUC_4C_8(S)$, $HAC_5C_6C_7[n, m]$ and $HAC_5C_7[n, m]$ having perfect and almost perfect H -packing and an induced H -packing k -Partition when $H \simeq P_3$ and $H \simeq C_4$ where P_3 is a path on three vertices and C_4 is a cycle on 4 vertices. Thus the study of partitioning a H -packing such that no two members in the same partition interfere, becomes meaningful. We define this concept as follows:

A collection $\mathcal{K} = \{H_1, H_2, \dots, H_r\}$ of induced subgraphs of a graph G is said to be *sg-independent* if (i) $V(H_i) \cap V(H_j) = \phi$, $i \neq j$, $1 \leq i, j \leq r$ and (ii) no edge of G has its one end in H_i and the other end in H_j , $i \neq j$, $1 \leq i, j \leq r$. If $H_i \simeq H$, $\forall i$, $1 \leq i \leq r$, then \mathcal{K} is referred to as a *H -independent set* of G . Let \mathcal{H} be a perfect or almost perfect H -packing of a graph G . Finding a partition $\{\mathcal{H}_1, \mathcal{H}_2, \dots, \mathcal{H}_k\}$ of \mathcal{H} such that \mathcal{H}_i is H -independent set, $\forall i$, $1 \leq i \leq k$, with minimum k is called the induced H -packing k -partition problem of G . The minimum induced H -packing k -partition number is denoted by $ipp_{\mathcal{H}}(G, H)$. The induced H -packing k -partition number denoted by $ipp(G, H)$ is defined as $ipp(G, H) = \min ipp_{\mathcal{H}}(G, H)$ where the minimum is taken over all H -packing of G [23].

The elementary concept and objective of the manuscript is to find H -packing and an induced H -packing k -partition number for certain nanostructures when $H \simeq P_3$ and $H \simeq C_4$. Hence we determine and investigate an P_3 -packing and an induced P_3 -packing k -partition number in section 2 for Armchair carbon nanotube $ACNT[n, m]$, in section 3 for Zigzag carbon nanotube $ZCNT[n, m]$, in section 4 for Zigzag polyhex nanotube $TUHC_6[2m, n]$, in section 5 for Boron triangular nanotubes $BNT_t[n, m]$, in section 6 for $TUC_4C_8(R)$ nanotube when $H \simeq P_3$ and C_4 , in section 7 for $TUC_4C_8(S)$ nanotube, in section 8 for $HAC_5C_6C_7[n, m]$ nanotube, and in section 9 for $HAC_5C_7[n, m]$ nanotube .

2 Armchair carbon nanotube

Carbon nanotubes consist of carbon atoms bonded into a tube shape where carbon atoms are located at apexes of regular hexagons on two-dimensional surfaces. There are different shapes of carbon nanotubes such as armchair, chiral and zigzag based on the rolling of $2D$ carbon hexagonal [5,10]. An armchair carbon nanotube of order

$n \times m$ is a tube obtained from a carbon hexagonal sheet of n rows and m columns by merging the vertices of last column with the respective vertices of first column and is denoted by $ACNT[n, m]$. $ACNT[n, m]$ has nm vertices, $\frac{m(3n-2)}{2}$ edges and has only odd number of rows and even number of columns. We investigate in this section on perfect and almost perfect P_3 -packing and an induced P_3 -packing k -partition number for armchair carbon nanotube.

Theorem 2.1 [25] *Let G be a graph and H be a subgraph of G . Then $\lambda(G, H) \leq \left\lfloor \frac{|V(G)|}{|V(H)|} \right\rfloor$.*

Packing with P_3 .

In view of Theorem 2.1 we have the following result.

Theorem 2.2 *Let G be a Armchair nanotube $ACNT[n, m]$ and $H \simeq P_3$, then $\lambda(G, P_3) \leq \left\lfloor \frac{nm}{3} \right\rfloor$.*

Lemma 2.3 *Let $G \simeq ACNT[3k + 1, 2]$, $k \geq 1$, $H \simeq P_3$. Then $\lambda(G, H) = \left\lfloor \frac{(3k + 1)}{2} \right\rfloor$.*

Proof We prove the result by induction on k . When $k = 1$, $\lambda(G, H) = 2$. See Fig. 1. Assume that $\lambda(ACNT(3k - 1, 2), H) = \left\lfloor \frac{(3k - 1)}{2} \right\rfloor$. Now $(ACNT[3k + 1, 2])$ is obtained by adding hexagon C_6 to $(ACNT[3k - 1, 2])$ sharing the top two vertices of $(ACNT[3k - 1, 2])$ that induce path P_3 .

Thus $\lambda(ACNT([3k + 1, 2], P_3) = \lambda(ACNT([3k - 1, 2], P_3) + 1 = \left\lfloor \frac{(3k - 1)}{2} \right\rfloor + 1 = \left\lfloor \frac{(3k + 1)}{2} \right\rfloor$. We proceed to prove that $\lambda(ACNT[n, m], P_3) = \left\lfloor \frac{nm}{3} \right\rfloor$. Let the subgraph induced by the vertices of columns j and $j + 1$ be denoted by A_j , $1 \leq j \leq m$.

Procedure Packing $(ACNT[n, m], P_3)$:

Input: An Armchair carbon nanotube $ACNT[n, m]$ and $H \simeq P_3$.

Algorithm:

- (i) Obtain a H -packing of A_1 as in Lemma 2.3. Then obtain a H -packing of A_3 by taking the mirror image of H -packing of A_1 , placing the mirror perpendicular to the horizontal edges of A_2 .
- (ii) Repeat step (i) for the subgraphs $A_j \cup A_{j+1} \cup A_{j+2} \cup \dots \cup A_m$, where $1 \leq j \leq m$.
- (iii) Obtain a H -packing of A_m as in A_1 when $m \equiv 0, 1, 2 \pmod{3}$.

Output: There exists a perfect and almost H -packing of armchair nanotube $ACNT[n, m]$ with $\left\lfloor \frac{nm}{3} \right\rfloor$ copies of H where $H \simeq P_3$.

Proof of correctness: In armchair nanotube $ACNT[n, m]$, the induced subgraphs A_j , $1 \leq j \leq m$ are vertex disjoint. The algorithm covers all vertices of $ACNT[n, m]$ when $m \equiv 0 \pmod{3}$ and leaves one or two vertices unsaturated when $m \equiv 1, 2 \pmod{3}$. Thus $\lambda(G, H) = \left\lfloor \frac{nm}{3} \right\rfloor$. \square

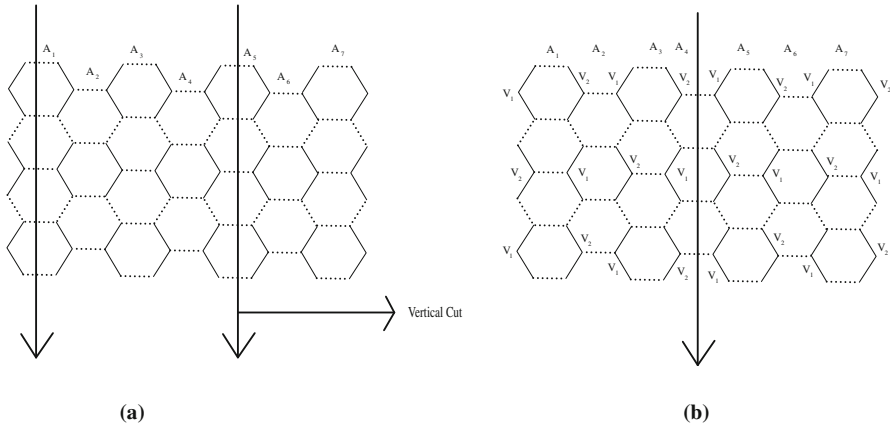


Fig. 1 **a** Induced P_3 -packing for $ACNT[9, 8]$, **b** Induced P_3 -packing 2 - partition for $ACNT[9, 8]$

Theorem 2.4 [29] *Let G be a graph which is connected, $|V(G)| > 3$ and if G has a perfect P_3 - Packing, then $ipp(G) > 1$.*

In view of Theorem 2.4 we have the following result.

Lemma 2.5 *The induced P_3 -packing k -partition number for armchair nanotube $ACNT[n, m]$ is 2.*

Let G be a armchair nanotube $ACNT[n, m]$. We now give a procedure and its proof of correctness to show that $ipp(ACNT[n, m], P_3) = 2$.

Procedure Partition for $(ACNT[n, m], P_3)$

Input: The armchair nanotube $ACNT[n, m]$ $ipp(G) = 2$.

Algorithm:

- (i) Consider any column of armchair nanotube $ACNT[n, m]$ and cut it vertically as in Fig. 1.
- (ii) Label P_3 -packing $[V_1]$ and $[V_2]$ in the sequence of consecutive packing starting at the top left most of the vertical plane.
- (iii) Label P_3 -packing $[V_2]$ and $[V_1]$ in the sequence of consecutive packing starting at the below left most of the vertical plane.
- (iv) Continue the process as in (ii) and (iii) for the sequence of consecutive columns, labelling $[V_1][V_2]$ or $[V_2][V_1]$ according as the label of $(m - 1)^{th}$ column is $[V_2][V_1]$ or $[V_1][V_2]$.

Output: Induced P_3 -packing k -partition number for armchair nanotube $ACNT[n, m]$ is 2.

Proof of correctness: Repeating the process of (iv) implies that there exists a induced P_3 -packing 2-partition number for armchair nanotube $ACNT[n, m]$. Hence $ipp(ACNT[n, m], P_3) = 2$.

3 Zigzag carbon nanotube

One of the shapes of carbon nanotubes is zigzag nanotube. The Zigzag carbon nanotube $ZCNT[n, m]$ has n rows and m columns. The Zigzag carbon nanotube has only even number of rows and even number of columns and it has nm vertices [20]. The Zigzag carbon nanotubes possess electrical properties similar to semiconductors. Armchair and Zigzag differ in chiral angle and diameter. We investigate in this section on perfect P_3 -packing and an induced P_3 -packing k -partition number for Zigzag carbon nanotube.

In view of Theorem 2.1 we have the following result.

Theorem 3.1 *Let G be a Zigzag carbon nanotube $ZCNT[n, m]$ and $H \simeq P_3$, then $\lambda(G, P_3) \leq \lfloor \frac{nm}{3} \rfloor$.*

Lemma 3.2 *Let $G \simeq ZCNT[3k + 1, 2]$, $k \geq 1$, $H \simeq P_3$. Then $\lambda(G, H) = (3k + 1)$.*

Proof We prove the result by induction on k . When $k = 1$, $\lambda(G, H) = 4$. See Fig. 2. Assume that $\lambda(ZCNT(3k - 1, 2), H) = (3k - 1)$. Now $ZCNT[3k + 1, 2]$ is obtained by adding 2 hexagons C_6 to $ZCNT[3k - 1, 2]$ sharing the vertices in $ZCNT[3k - 1, 2]$ that induce path P_3 .

Thus $\lambda(ZCNT([3k + 1, 2], P_3) = \lambda(ZCNT([3k - 1, 2], P_3) + 2 = (3k - 1) + 2 = (3k + 1)$.

We proceed to prove that $\lambda(ZCNT[n, m], P_3) = \lfloor \frac{nm}{3} \rfloor$. Let the subgraph induced by the vertices of rows i and $i + 1$ be denoted by A_i , $1 \leq i \leq n$.

Procedure Packing $(ZCNT[n, m], P_3)$:

Input: An Zigzag carbon nanotube $ZCNT[n, m]$ and $H \simeq P_3$.

Algorithm:

- (i) Obtain a H -packing of A_1 as in Lemma 3.2. Then obtain a H -packing of A_3 by taking the mirror image of H -packing of A_1 , placing the mirror perpendicular to the obtuse, acute edges of A_2 .
- (ii) Repeat step (i) for the subgraphs $A_i \cup A_{i+1} \cup A_{i+2} \cup \dots \cup A_n$ where $1 \leq i \leq n$.
- (iii) Obtain a H -packing of A_m as in A_1 when $n \equiv 0 \pmod{3}$.

Output: There exists a perfect H -packing of Zigzag nanotube $ZCNT[n, m]$ with $\lfloor \frac{nm}{3} \rfloor$ copies of H where $H \simeq P_3$.

Proof of correctness: In Zigzag nanotube $ZCNT[n, m]$, the induced subgraphs A_i , $1 \leq i \leq n$ are vertex disjoint. The algorithm covers all vertices of $ZCNT[n, m]$ when $n \equiv 0 \pmod{3}$. Thus $\lambda(G, H) = \lfloor \frac{nm}{3} \rfloor$. \square

Lemma 3.3 *The induced P_3 -packing k -partition number for Zigzag nanotube $ZCNT[n, m]$ is 2.*

Proof Let G be a Zigzag nanotube $ZCNT[n, m]$. We now give a procedure and its proof of correctness to show that $ipp(ZCNT[n, m], P_3) = 2$.

Procedure Partition for $(ZCNT[n, m], P_3)$

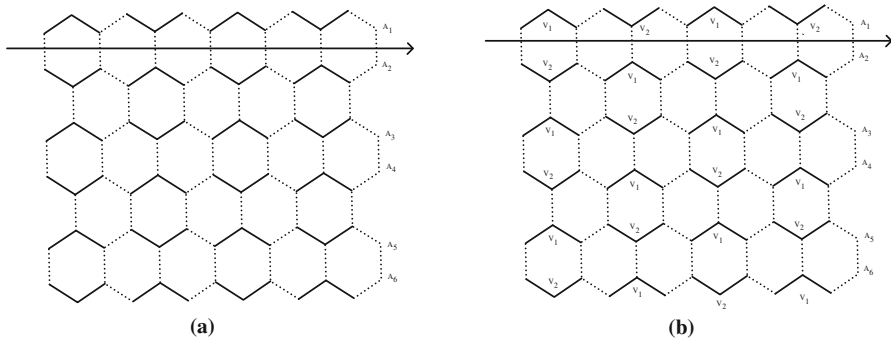


Fig. 2 a Induced P_3 -packing for $ZCNT[6, 12]$ b Induced P_3 -packing 2 - partition for $ZCNT[6, 12]$

Input: The Zigzag nanotube $ZCNT[n, m]$ $ipp(G) = 2$.

Algorithm:

- (i) Consider any row of Zigzag nanotube $ZCNT[n, m]$ and cut it horizontally as in Fig. 2.
- (ii) Label P_3 -packing $[V_1]$ and $[V_2]$ in the sequence of consecutive packing starting at the top left most of the horizontal plane.
- (iii) Label P_3 -packing $[V_2]$ and $[V_1]$ in the sequence of consecutive packing starting at the below left most of the horizontal plane.
- (iv) Continue the process as in (ii) and (iii) for the sequence of consecutive rows, labelling $[V_1]$ $[V_2]$ or $[V_2]$ $[V_1]$ according as the label of $(n - 1)^{th}$ row is $[V_2]$ $[V_1]$ or $[V_1]$ $[V_2]$.

Output: Induced P_3 -packing k -partition number for Zigzag nanotube $ZCNT[n, m]$ is 2.

Proof of correctness: Repeating the process of (iv) implies that there exists an induced P_3 -packing 2-partition number for Zigzag nanotube $ZCNT[n, m]$. Hence $ipp(ZCNT[n, m], P_3) = 2$. □

4 Zigzag polyhex carbon nanotube $TUHC_6[2m, n]$

The structure $TUHC_6[2m, n]$ has $2nm$ vertices and $3nm - n$ edges, where n is the number of rows and m is the number of columns. The $TUHC_6[2m, n]$ nanotube is known as Zigzag polyhex nanotube with circumference $2m$ and length n and it is a bi-regular graph [6,24]. We investigate in this section on perfect and almost perfect P_3 -packing and an induced P_3 -packing k -partition number for $TUHC_6[2m, n]$ carbon nanotube.

In view of Theorem 2.1 we have the following result.

Theorem 4.1 Let G be a $TUHC_6[2m, n]$ nanotube and $H \simeq P_3$, then $\lambda(G, P_3) \leq \lfloor \frac{2nm}{3} \rfloor$.

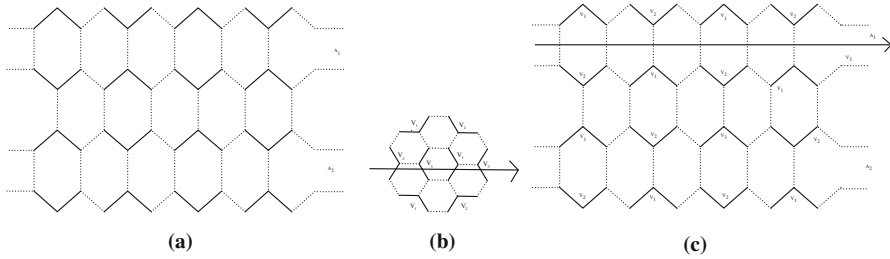


Fig. 3 a Induced P_3 -packing for $TUHC_6[6, 4]$ b P_3 -packing 3 - partition for induced subgraph of $TUHC_6[6, 4]$ c Induced P_3 -packing 3 - partition for $TUHC_6[6, 4]$

Lemma 4.2 Let $G \simeq TUHC_6[2k + 1, 4]$, $k \geq 1$, $H \simeq P_3$. Then $\lambda(G, H) = \lfloor \frac{8}{3}(2k + 1) \rfloor$.

Proof We prove the result by induction on k . When $k = 1$, $\lambda(G, H) = 8$. See Fig. 3. Assume that $\lambda(TUHC_6[2k - 1, 4], H) = \lfloor \frac{8}{3}(2k - 1) \rfloor$. Now $(TUHC_6[2k + 1, 4])$ is obtained by adding hexagons C_6 of 2 copies $(TUHC_6[2k - 1, 4])$ to $(TUHC_6[2k - 1, 4])$ that induce path P_3 .

$$\text{Thus } \lambda(TUHC_6[2k + 1, 4], P_3) = \lambda(TUHC_6[2k - 1, 4], P_3) + 2 = \lfloor \frac{8}{3}(2k - 1) \rfloor + 2 = \lfloor \frac{8}{3}(2k + 1) \rfloor.$$

We proceed to prove that $\lambda(TUHC_6[2m, n], P_3) = \lfloor \frac{2nm}{3} \rfloor$. Let the subgraph induced by the vertices of rows i and $i + 1$ be denoted by A_i , $1 \leq i \leq n$.

Procedure Packing $(TUHC_6[2m, n], P_3)$:

Input: The Zigzag polyhex carbon nanotube $TUHC_6[2m, n]$ and $H \simeq P_3$.

Algorithm:

- (i) Obtain a H -packing of A_1 as in Lemma 4.2. Then obtain a H -packing of A_2 by taking the mirror image of H -packing of A_1 , placing the mirror horizontal to A_1 and joining vertical edge between A_1 A_2 .
- (ii) Repeat step (i) for the subgraphs $A_i \cup A_{i+1} \cup A_{i+2} \cup \dots \cup A_n$ where $1 \leq i \leq n$.
- (iii) Obtain a H -packing of A_n as in A_1 when $n \equiv 0, 1, 2 \pmod{3}$.

Output: There exists perfect and almost perfect H -packing of nanotube $TUHC_6[2m, n]$ with $\lfloor \frac{2nm}{3} \rfloor$ copies of H where $H \simeq P_3$.

Proof of correctness: In nanotube $TUHC_6[2m, n]$, the induced subgraphs A_i , $1 \leq i \leq n$ are vertex disjoint. The algorithm covers all vertices of $TUHC_6[2m, n]$ when $n \equiv 0 \pmod{3}$ and leaves one or two vertices unsaturated when $n \equiv 1, 2 \pmod{3}$.

$$\text{Thus } \lambda(G, H) = \lfloor \frac{2nm}{3} \rfloor.$$

Lemma 4.3 The induced P_3 -packing k -partition number for $TUHC_6[2m, n]$ nanotube is 3.

Proof Let G be a $TUHC_6[2m, n]$ nanotube. We now give a procedure and its proof of correctness to show that $ipp(TUHC_6[2m, n], P_3) = 3$.

Procedure Partition for $(TUHC_6[2m, n], P_3)$

Input: The Zigzag polyhex carbon nanotube $TUHC_6[2m, n]$ $ipp(G) = 3$.

Algorithm:

- (i) Consider any row of $TUHC_6[2m, n]$ and cut it horizontally as in Fig. 3.
- (ii) Choose a P_3 path on 3 vertices as shown in Fig. 3. The adjacent vertices of V_1 cannot be partitioned into V_2 alone. It fails the definition of induced P_3 -packing k -partition.
- (iii) Start a path of P_3 -packing of V_1 -partition. The adjacent path of partition of V_1 is either V_2 or V_3 .
- (iv) Start a path of P_3 -packing of V_2 -partition. The adjacent path of partition of V_2 is either V_3 or V_1 .
- (v) Construct a path of P_3 -packing of V_3 -partition. The adjacent path of partition of V_3 is either V_2 or V_1 .
- (vi) Continue the process of (iii), (iv) and (v) where all the vertices are covered and partitioned into 3-partition.

Output: Induced P_3 -packing k -partition number for $TUHC_6[2m, n]$ nanotube is 3.

Proof of correctness: Repeating the process (vi) implies, that there exists induced perfect P_3 -packing 3-partition for $TUHC_6[2m, n]$ nanotube. \square

5 Boron triangular carbon nanotube $BNT_t[n, m]$

Boron nanotubes are becoming increasingly interesting because of their remarkable properties, such as their structural stability, work function, transport properties, and electronic structure [19]. A boron triangular sheet is obtained from a carbon hexagonal sheet by adding an extra atom to the center of each hexagon. Boron nanomaterials have been considered as excellent materials for enhancing the characteristics of optoelectronic nanodevices because of their broad elastic modulus, high-melting point, excessive conductivity, great emission uniformity, and low turn-on field. These materials can carry excessive emission current, which recommends that they may have great prospective applications in the field emission area [17]. Scientists believe that boron triangular nanotubes are a better conductor than carbon hexagonal nanotubes. $BNT_t[n, m]$ of order $n \times m$, where n and m represent the number of items in each row and each column, respectively. There are $\frac{3nm}{2}$ vertices and $\frac{3m(3n-2)}{2}$ edges in the boron triangular nanotubes. We investigate in this section on perfect and almost perfect P_3 -packing and an induced P_3 -packing k -partition number for $BNT_t[n, m]$ carbon nanotube.

In view of Theorem 2.1 we have the following result.

Theorem 5.1 Let G be a $BNT_t[n, m]$ nanotube and $H \simeq P_3$, then $\lambda(G, P_3) \leq \left\lfloor \frac{nm}{2} \right\rfloor$.

Lemma 5.2 Let $G \simeq BNT_t[2k+1, 2]$, $k \geq 1$, $H \simeq P_3$. Then $\lambda(G, H) = (2k+1)$.

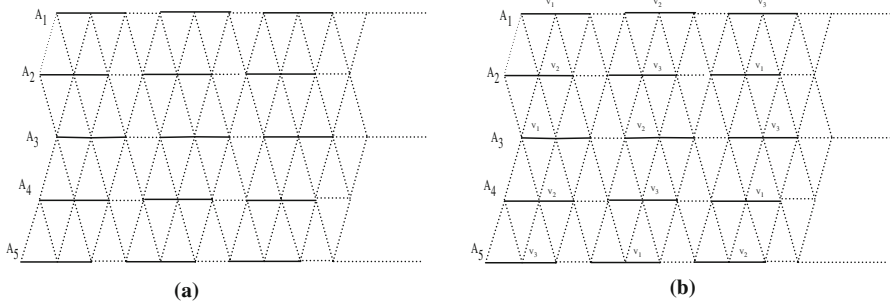


Fig. 4 (a) Induced P_3 -packing for $BNT[5, 6]$ (b) Induced P_3 -packing 3-partition for $BNT[5, 6]$

Proof We prove the result by induction on k . When $k = 1$, $\lambda(G, H) = 3$. See Fig. 4. Assume that $\lambda(BNT_t(2k - 1, 2), H) = (2k - 1)$. Now $(BNT_t[2k + 1, 2])$ is obtained by adding k_3 of two copies $(BNT_t[2k - 1, 2])$ to $(BNT_t[2k - 1, 2])$ joining all the edges from the middle vertices that induce the path P_3 .

Thus $\lambda(BNT_t([2k + 1, 2], P_3)) = \lambda(BNT_t([2k - 1, 2], P_3)) + 2 = (2k - 1) + 2 = (2k + 1)$.

We proceed to prove that $\lambda(BNT_t[n, m], P_3) = \lfloor \frac{nm}{2} \rfloor$. Let the subgraph induced by the vertices of rows i and $i + 1$ be denoted by A_i , $1 \leq i \leq n$.

Procedure Packing $(BNT_t[n, m], P_3)$:

Input: The Boron triangular nanotube $BNT_t[n, m]$ and $H \simeq P_3$.

Algorithm:

- (i) Obtain a H -packing of A_1 as in Lemma 5.2. Then obtain a H -packing of A_2 by taking the mirror image of H -packing of A_1 , placing the mirror horizontal to the obtuse and acute edges from A_1 .
- (ii) Repeat step (i) for the subgraphs $A_i \cup A_{i+1} \cup A_{i+2} \cup \dots \cup A_n$, where $1 \leq i \leq n$.
- (iii) Obtain a H -packing of A_n as in A_1 when $n \equiv 0, 1, 2 \pmod{3}$.

Output: There exists perfect and almost perfect H -packing of nanotube $BNT_t[n, m]$ with $\lfloor \frac{nm}{2} \rfloor$ copies of H where $H \simeq P_3$.

Proof of correctness: In nanotube $BNT_t[n, m]$, the induced subgraphs A_i , $1 \leq i \leq n$ are vertex disjoint. The algorithm covers all vertices of $BNT_t[n, m]$ when $n \equiv 0 \pmod{3}$ and leaves one or two vertices unsaturated when $n \equiv 1, 2 \pmod{3}$. Thus $\lambda(G, H) = \lfloor \frac{nm}{2} \rfloor$.

Lemma 5.3 The induced P_3 -packing k -partition number for $BNT_t[n, m]$ nanotube is 3.

Proof Let G be a $BNT_t[n, m]$ nanotube. We now give a procedure and its proof of correctness to show that $ipp(BNT_t[n, m], P_3) = 3$.

Procedure Partition for $(BNT_t[n, m], P_3)$

Input: The Boron triangular carbon nanotubes $BNT_t[n, m]$ $ipp(G) = 3$.

Algorithm:

- (i) Consider any row A_1 of $BNT_t[n, m]$ and cut it horizontally as in Fig. 4.
- (ii) Label P_3 -packing of A_1 as $[V_1], [V_2]$ and $[V_3]$ starting at the top left most of horizontal plane.
- (iii) Label P_3 -packing of A_1 as $[V_2], [V_3]$ and $[V_1]$ starting at the below left most of horizontal plane.
- (iv) A_2 is labeled as $[V_1], [V_2], [V_3]$ or $[V_2], [V_3], [V_1]$ or $[V_3], [V_1], [V_2]$ or $[V_3], [V_2], [V_1]$ etc. . . according to the labeling of A_1 .
- (v) Continue as in (iv) for A_3, A_4, \dots, A_n till it is possible to find 3-partition in G .

Output:

There exists an induced H -packing 3-partition for $BNT_t[n, m]$ nanotube.

Proof of Correctness: The labeling process of (i) to (v) in algorithm implies that it is possible to pack the $BNT_t[n, m]$ nanotube with 3-partition. Hence $ipp(G) = 3$. □

6 $TUC_4C_8(S)$ carbon nanotube

The structure $TUC_4C_8(S)$ has $8nm$ vertices and $12nm - 2m$ edges, where n is the number of rows and m is the number of columns. The $TUC_4C_8(S)$ nanotube is bi-regular graph [24]. We investigate in this section on perfect and almost perfect P_3 -packing and an induced P_3 -packing k -partition number for $TUC_4C_8(S)$ carbon nanotube, where n is the number of octagons in each row and m is the number of octagons in each column, where n and m are positive integers.

In view of Theorem 2.1 we have the following result.

Theorem 6.1 *Let G be a $TUC_4C_8(S)$ nanotube and $H \simeq P_3$, then $\lambda(G, P_3) \leq \lfloor \frac{8nm}{3} \rfloor$.*

Lemma 6.2 *Let $G \simeq TUC_4C_8(S)[2k + 1, 3]$, $k \geq 1$, $H \simeq P_3$. Then $\lambda(G, H) = 8(2k + 1)$.*

Proof We prove the result by induction on k . When $k = 1$, $\lambda(G, H) = 24$. See Fig. 5. Assume that $\lambda(TUC_4C_8(S)(2k - 1, 3), H) = 8(2k - 1)$. Now $(TUC_4C_8(S)(2k + 1, 3))$ is obtained by adding C_4C_8 of two copies $(TUC_4C_8(S)(2k - 1, 3))$ to $(TUC_4C_8(S)(2k - 1, 3))$ sharing the vertices in $(TUC_4C_8(S)(2k - 1, 3))$ that induce the path P_3 . Thus $\lambda((TUC_4C_8(S)(2k + 1, 3), P_3) = \lambda((TUC_4C_8(S)(2k - 1, 3), P_3) + 2 = 8(2k - 1) + 2 = 8(2k + 1)$.

We proceed to prove that $\lambda(TUC_4C_8(S), P_3) = \lfloor \frac{8nm}{3} \rfloor$. Let the subgraph induced by the vertices of columns j and $j + 1$ be denoted by A_j , $1 \leq j \leq m$.

Procedure Packing $(TUC_4C_8(S), P_3)$:

Input: The Carbon nanotube $TUC_4C_8(S)$ and $H \simeq P_3$.

Algorithm:

- (i) Obtain a H -packing of A_1 as in Lemma 6.2. Then obtain a H -packing of A_2 by taking the mirror image of H -packing of A_1 , placing the mirror perpendicular to A_1 and joining A_1 and A_2 by an horizontal edges.

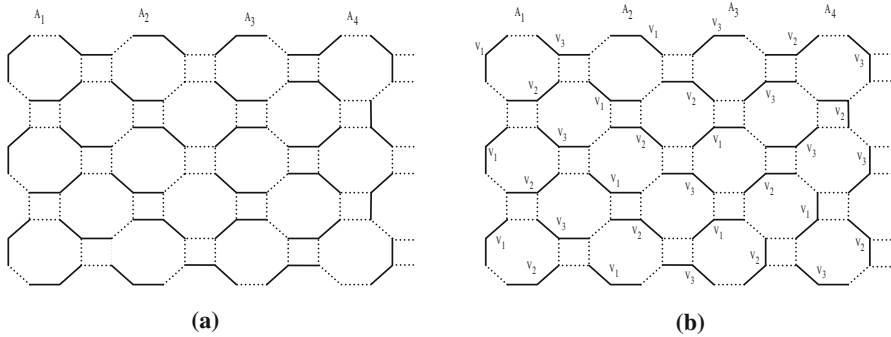


Fig. 5 **a** Induced P_3 -packing for $TUC_4C_8(S)[4, 3]$, **b** Induced P_3 -packing 3 - partition for $TUC_4C_8(S)[4, 3]$

- (ii) Repeat step (i) for the subgraphs $A_j \cup A_{j+1} \cup A_{j+2} \cup \dots \cup A_m$, where $1 \leq j \leq m$.
- (iii) Obtain a H -packing of A_m as in A_1 when $m \equiv 0, 1, 2 \pmod{3}$.

Output: There exists perfect and almost perfect H -packing of nanotube $TUC_4C_8(S)$ with $\lfloor \frac{8nm}{3} \rfloor$ copies of H where $H \simeq P_3$.

Proof of correctness: In Carbon nanotube $TUC_4C_8(S)$, the induced subgraphs A_j , $1 \leq j \leq m$ are vertex disjoint. The algorithm covers all vertices of $TUC_4C_8(S)[n, m]$ when $m \equiv 0 \pmod{3}$ and leaves one or two vertices unsaturated when $m \equiv 1, 2 \pmod{3}$. Thus $\lambda(G, H) = \lfloor \frac{8nm}{3} \rfloor$. \square

Lemma 6.3 The induced P_3 -packing k -partition number for $TUC_4C_8(S)$ is 3.

Procedure Partition for $(TUC_4C_8(S), P_3)$

Input: The induced P_3 -packing k -partition number for $TUC_4C_8(S)$ nanotube is 3.

Algorithm:

- (i) Choose a P_3 path on 3 vertices in A_1, A_2, \dots as in Fig. 5. The adjacent vertices of V_1 cannot be partitioned into V_2 alone. It fails the definition of induced P_3 -packing k -partition.
- (ii) Start a path of P_3 -packing of V_1 -partition. The adjacent path of partition of V_1 is either V_2 or V_3 .
- (iii) Start a path of P_3 -packing of V_2 -partition. The adjacent path of partition of V_2 is either V_3 or V_1 .
- (iv) Construct a path of P_3 -packing of V_3 -partition. The adjacent path of partition of V_3 is either V_2 or V_1 .
- (v) Continue the process of (ii), (iii) and (iv) where all the vertices are covered and partitioned into 3-partition.

Output: Induced P_3 -packing k -partition number for $TUC_4C_8(S)$ nanotube is 3.

Proof of correctness: Repeating the process (v) implies, that there exists induced P_3 -packing 3-partition for $TUC_4C_8(S)$ nanotube.

7 $TUC_4C_8(R)$ carbon nanotube

$TUC_4C_8(R)$ has $4pq$ vertices and $6pq - p$ edges, where n and m denote the number of squares in a row and the number of rows of squares respectively [22]. We investigate in this section on perfect and almost perfect P_3 -packing and an induced P_3 -packing k -partition number for $TUC_4C_8(R)$ carbon nanotube, where n is the number of octagons in each row and m is the number of octagons in each column, where n and m are positive integers. Further in this section, we prove that perfect C_4 -packing 2-partition exists for $TUC_4C_8(R)$ nanotube.

In view of Theorem 2.1 we have the following result.

Theorem 7.1 *Let G be a $TUC_4C_8(R)$ nanotube and $H \simeq P_3$, then $\lambda(G, P_3) \leq \lfloor \frac{4pq}{3} \rfloor$.*

Lemma 7.2 *Let $G \simeq TUC_4C_8(R)[2k + 1, 3]$, $k \geq 1$, $H \simeq P_3$. Then $\lambda(G, H) = 4(2k + 1)$.*

Proof We prove the result by induction on k . When $k = 1$, $\lambda(G, H) = 12$. See Fig. 6. Assume that $\lambda(TUC_4C_8(R)(2k - 1, 3), H) = 4(2k - 1)$. Now $(TUC_4C_8(R)(2k + 1, 3))$ is obtained by adding squares of two copies $(TUC_4C_8(R)(2k - 1, 3))$ to $(TUC_4C_8(R)(2k - 1, 3))$ sharing the vertices in $(TUC_4C_8(R)(2k - 1, 3))$ that induce the path P_3 .

Thus $\lambda((TUC_4C_8(R)(2k + 1, 3), P_3) = \lambda((TUC_4C_8(R)(2k - 1, 3), P_3) + 2 = 4(2k - 1) + 2 = 4(2k + 1)$.

We proceed to prove that $\lambda(TUC_4C_8(R), P_3) = \lfloor \frac{4pq}{3} \rfloor$. Let the subgraph induced by the vertices of rows i and $i + 1$ be denoted by A_i , $1 \leq i \leq n$.

Procedure Packing $(TUC_4C_8(R), P_3)$:

Input: The Carbon nanotube $TUC_4C_8(R)$ and $H \simeq P_3$.

Algorithm:

- (i) Obtain a H -packing of A_1 as in Lemma 7.2. Then obtain a H -packing of A_3 by taking the mirror image of H -packing of A_1 , placing the mirror horizontal to the vertical edges of A_2 .

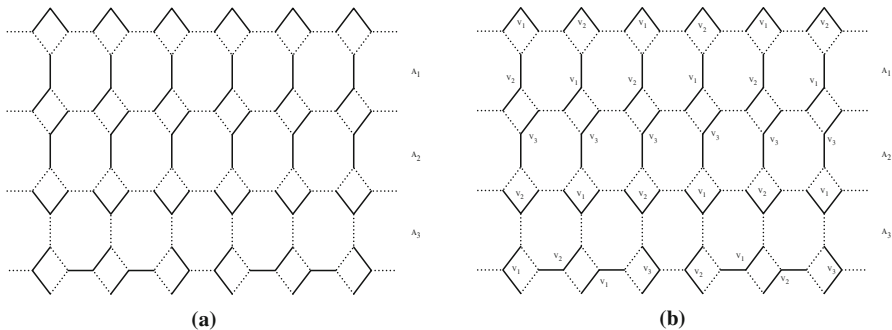


Fig. 6 **a** Induced P_3 -packing for $TUC_4C_8(R)[6,4]$, **b** Induced P_3 -packing 3 - partition for $TUC_4C_8(R)[6,4]$

- (ii) Repeat step (i) for the subgraphs $A_i \cup A_{i+1} \cup A_{i+2} \cup \dots \cup A_n$ where $1 \leq i \leq n$.
 (iii) Obtain a H -packing of A_n as in A_1 when $n \equiv 0, 1, 2 \pmod{3}$.

Output: There exists perfect and almost perfect H -packing of nanotube $TUC_4C_8(R)$ with $\lfloor \frac{4pq}{3} \rfloor$ copies of H where $H \simeq P_3$.

Proof of correctness: In nanotube $TUC_4C_8(R)[n, m]$, the induced subgraphs A_i , $1 \leq i \leq n$ are vertex disjoint. The algorithm covers all vertices of $TUC_4C_8(R)$ when $n \equiv 0 \pmod{3}$ and leaves one or two vertices unsaturated when $n \equiv 1, 2 \pmod{3}$.

Thus $\lambda(G, H) = \lfloor \frac{4pq}{3} \rfloor$. \square

Lemma 7.3 *The induced P_3 -packing k -partition number for $(TUC_4C_8(R))$ nanotube is 3.*

Proof Let G be a $TUC_4C_8(R)$ nanotube. We now give a procedure and its proof of correctness to show that $ipp(TUC_4C_8(R), P_3) = 3$.

Procedure Partition for $(TUC_4C_8(R), P_3)$

Input: The induced P_3 -packing k -partition number for $TUC_4C_8(R)$ nanotube is 3.

Algorithm:

- (i) Consider A_1 and label P_3 -packing as in Fig. 6.
- (ii) Label P_3 -packing of A_1 as $[V_1]$ and $[V_2]$ or $[V_2]$ and $[V_1]$ starting at the top left most of horizontal plane.
- (iii) Label P_3 -packing of A_2 as $[V_3]$ and $[V_2]$ and $[V_1]$ starting at the below left most of horizontal plane.
- (iv) A_3 is labeled as $[V_1]$, $[V_2]$ or $[V_2]$, $[V_1]$, or $[V_1]$, $[V_2]$, $[V_3]$ or $[V_2]$, $[V_3]$, $[V_1]$ or $[V_3]$, $[V_1]$, $[V_2]$ etc. . . according to the labeling of A_2 .
- (v) Continue as in (iv) for A_4, A_5, \dots, A_n till it is possible to find 3-partition in G .

Output:

There exists an induced P_3 -packing 3-partition for $TUC_4C_8(R)$ nanotube.

Proof of Correctness: The labeling process of (ii) to (v) in algorithm implies that it is possible to pack the $TUC_4C_8(R)$ nanotube with 3-partition. Hence $ipp(G) = 3$. \square

In view of Theorem 2.1 we have the following result.

Theorem 7.4 *Let G be a $TUC_4C_8(R)[n, m]$ nanotube and $H \simeq C_4$, then $\lambda(G, C_4) \leq pq$.*

Lemma 7.5 *Let $G \simeq TUC_4C_8(R)[2k + 1, 2]$, $k \geq 1$, $H \simeq C_4$. Then $\lambda(G, H) = 2(2k + 1)$.*

Proof We prove the result by induction on k . When $k = 1$, $\lambda(G, H) = 6$. See Fig. 7. Assume that $\lambda(TUC_4C_8(R)(2k - 1, 2), H) = 2(2k - 1)$. Now $(TUC_4C_8(R)(2k + 1, 2))$ is obtained by adding C_4C_8 of two copies $(TUC_4C_8(R)(2k - 1, 2))$ to $(TUC_4C_8(R)(2k - 1, 2))$ sharing the vertices in $(TUC_4C_8(R)(2k - 1, 2))$ that induce the cycle C_4 .

Thus $\lambda(TUC_4C_8(R)(2k + 1, 2), C_4) = \lambda(TUC_4C_8(R)(2k - 1, 2), C_4) + 2 = 2(2k - 1) + 2 = 2(2k + 1)$.

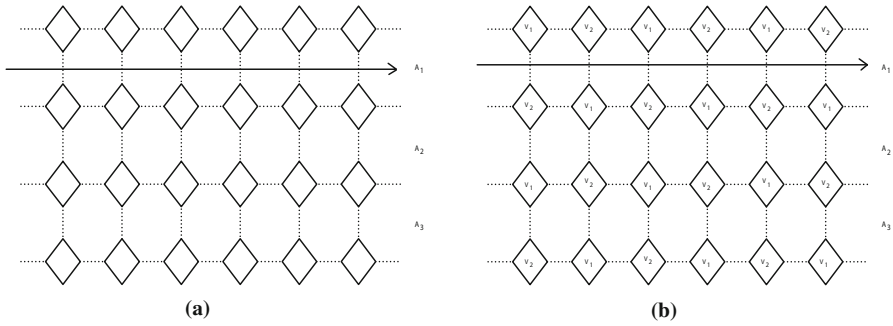


Fig. 7 **a** Induced C_4 -packing for $TUC_4C_8(R)[6,4]$, **b** Induced C_4 -packing 2 - partition for $TUC_4C_8(R)[6,4]$

We proceed to prove that $\lambda(TUC_4C_8(R), C_4) = pq$. Let the subgraph induced by the vertices of rows i and $i + 1$ be denoted by $A_i, 1 \leq i \leq n$.

Procedure Packing $(TUC_4C_8(R), C_4)$:

Input: The nanotube $TUC_4C_8(R)$ and $H \simeq C_4$.

Algorithm:

- (i) Obtain a H -packing of A_1 as in Lemma 7.5. Then obtain a H -packing of A_3 by taking the mirror image of H -packing of A_1 , placing the mirror horizontal to the vertical edges of A_2 .
- (ii) Repeat step (i) for the subgraphs $A_i \cup A_{i+1} \cup A_{i+2} \cup \dots \cup A_n$, where $1 \leq i \leq n$.
- (iii) Obtain a H -packing of A_n as in A_1 when $n \equiv 0 \pmod{3}$.

Output: There exists perfect H -packing of nanotube $TUC_4C_8(R)[n, m]$ with pq copies of H where $H \simeq C_4$.

Proof of correctness: In nanotube $TUC_4C_8(R)[n, m]$, the induced subgraphs $A_i, 1 \leq i \leq n$ are vertex disjoint. The algorithm covers all vertices of $TUC_4C_8(R)[n, m]$ when $n \equiv 0 \pmod{3}$. Thus $\lambda(G, H) = pq$. □

Lemma 7.6 *The induced C_4 -packing k -partition number for $(TUC_4C_8(R))$ nanotube is 2.*

Proof Let G be a $(TUC_4C_8(R))$ nanotube. We now give a procedure and its proof of correctness to show that $ipp(TUC_4C_8(R)[n, m], C_4) = 2$.

Procedure Partition for $(TUC_4C_8(R), C_4)$

Input: The Induced C_4 -packing k -partition number for $TUC_4C_8(R)$ nanotube is 2.

Algorithm:

- (i) Consider any row of $(TUC_4C_8(R))$ nanotube and cut it horizontally as in Fig. 7.
- (ii) Label C_4 -packing $[V_1]$ and $[V_2]$ in the sequence of consecutive packing starting at the top left most of the horizontal plane.
- (iii) Label C_4 -packing $[V_2]$ and $[V_1]$ in the sequence of consecutive packing starting at the below left most of the horizontal plane.
- (iv) Continue the process as in (ii) and (iii) for the sequence of consecutive rows, labelling $[V_1]$ $[V_2]$ or $[V_2]$ $[V_1]$ according as the label of $(n - 1)^{th}$ row is $[V_2]$ $[V_1]$ or $[V_1]$ $[V_2]$.

Output: Induced C_4 -packing k -partition number for $(TUC_4C_8(R)[n, m])$ nanotube is 2.

Proof of correctness: Repeating the process of (iv) implies that there exists a Induced C_4 -packing 2-partition number for $(TUC_4C_8(R))$ nanotube. Hence $ipp((TUC_4C_8(R), C_4) = 2$. \square

8 $HAC_5C_6C_7[n, m]$ carbon nanotube

$HAC_5C_6C_7[n, m]$ is constructed by alternating C_5 , C_6 and C_7 carbon cycles. It is tube shaped material but we consider it in the form of sheet shown in Fig. 8. The number of pentagons in the first row is denoted by n . In $HAC_5C_6C_7[n, m]$, the three first rows of vertices and edges are repeated alternatively, and the number of this repetition denoted by m . In each phase there are $16n$ vertices and $2n$ vertices which are joined to the end of the graph and hence the number of vertices in this nanotube is equal to $16nm + 2n$ [15]. In this section we compute the perfect P_3 -packing and an induced P_3 -packing k -partition number for $HAC_5C_6C_7[n, m]$ nanotube.

In view of Theorem 2.1 we have the following result.

Theorem 8.1 Let G be a $HAC_5C_6C_7[n, m]$ nanotube and $H \simeq P_3$, then $\lambda(G, P_3) \leq \left\lfloor \frac{16nm + 2n}{3} \right\rfloor$.

Lemma 8.2 Let $G \simeq HAC_5C_6C_7[3, k + 1]$, $k \geq 1$, $H \simeq P_3$. Then $\lambda(G, H) = 17(k + 1)$.

Proof We prove the result by induction on k . When $k = 1$, $\lambda(G, H) = 34$. See Fig. 8. Assume that $\lambda(HAC_5C_6C_7[3, k - 1], H) = 17(k - 1)$. Now $HAC_5C_6C_7[3, k + 1]$ is obtained by adding two phases $C_5 C_6 C_7$ to $HAC_5C_6C_7[3, k - 1]$ that induce the path P_3 .

Thus $\lambda(HAC_5C_6C_7[3, k + 1], P_3) = \lambda(HAC_5C_6C_7[3, k - 1], P_3) + 2 = 17(k - 1) + 2 = 17(k + 1)$.

We proceed to prove that $\lambda(HAC_5C_6C_7[n, m], P_3) = \left\lfloor \frac{(16nm + 2n)}{3} \right\rfloor$. Let the subgraph induced by the vertices of rows i and $i + 1$ be denoted by A_i , $1 \leq i \leq n$.

Procedure Packing $(HAC_5C_6C_7[n, m], P_3)$:

Input: The nanotube $(HAC_5C_6C_7[n, m])$ and $H \simeq P_3$.

Algorithm:

- (i) Obtain a H -packing of A_1 as in Lemma 8.2. Then obtain a H -packing of A_2 by taking the mirror image of H -packing of A_1 , placing the mirror horizontal to A_1 , and joining an edge from A_1 .
- (ii) Repeat step (i) for the subgraphs $A_i \cup A_{i+1} \cup A_{i+2} \cup \dots \cup A_n$ where $1 \leq i \leq n$.
- (iii) Obtain a H -packing of A_n as in A_1 when $n \equiv 0 \pmod{3}$.

Output: There exists perfect H -packing of nanotube $HAC_5C_6C_7[n, m]$, with $\left\lfloor \frac{(16nm + 2n)}{3} \right\rfloor$ copies of H where $H \simeq P_3$.

Proof of correctness: In nanotube $HAC_5C_6C_7[n, m]$, the induced subgraphs

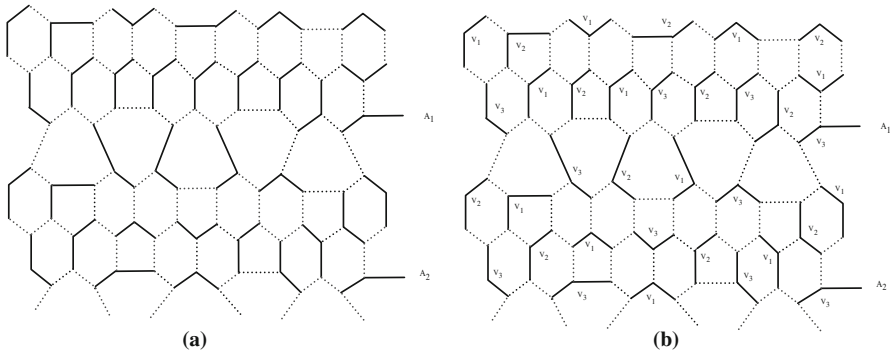


Fig. 8 **a** Induced P_3 -packing for $HAC_5C_6C_7[n, m]$, **b** Induced P_3 -packing 3 - partition for $HAC_5C_6C_7[n, m]$

$A_i, 1 \leq i \leq n$ are vertex disjoint. The algorithm covers all vertices of $HAC_5C_6C_7[n, m]$ when $n \equiv 0 \pmod{3}$. Thus $\lambda(G, H) = \left\lfloor \frac{(16mn + 2n)}{3} \right\rfloor$. \square

Lemma 8.3 *The induced P_3 -packing k -partition number for $HAC_5C_6C_7[n, m]$ nanotube is 3.*

Proof Let G be a $HAC_5C_6C_7[n, m]$ nanotube. We now give a procedure and its proof of correctness to show that $ipp(HAC_5C_6C_7[n, m], P_3) = 3$.

Procedure Partition for $(HAC_5C_6C_7[n, m], P_3)$

Input: The Induced P_3 -packing k -partition number for $HAC_5C_6C_7[n, m]$ nanotube is 3.

Algorithm:

- (i) Consider A_1 and label P_3 -packing as in Fig. 8.
- (ii) Label P_3 -packing of A_1 as $[V_1]$ and $[V_2]$ or $[V_2]$ and $[V_1]$ or $[V_3], [V_1]$ and $[V_2]$ or $[V_1], [V_3]$ and $[V_2]$ or $[V_2], [V_3]$ and $[V_1]$ starting at the top left most of horizontal plane.
- (iii) Label P_3 -packing of A_2 as $[V_2], [V_1]$ and $[V_3]$ or $[V_1], [V_3]$ and $[V_2]$ or $[V_3], [V_2]$ and $[V_1]$ etc. . . starting at the below left most of horizontal plane, according to the labeling of A_1 .
- (v) Continue as in (ii) and (iii) for A_3, A_4, \dots, A_n till it is possible to find 3-partition in G .

Output:

There exists an induced P_3 -packing 3-partition for $HAC_5C_6C_7[n, m]$ nanotube .

Proof of Correctness: The labeling process of (ii) to (iii) in algorithm implies that it is possible to pack the $HAC_5C_6C_7[n, m]$ nanotube with 3-partition. Hence $ipp(G) = 3$. \square

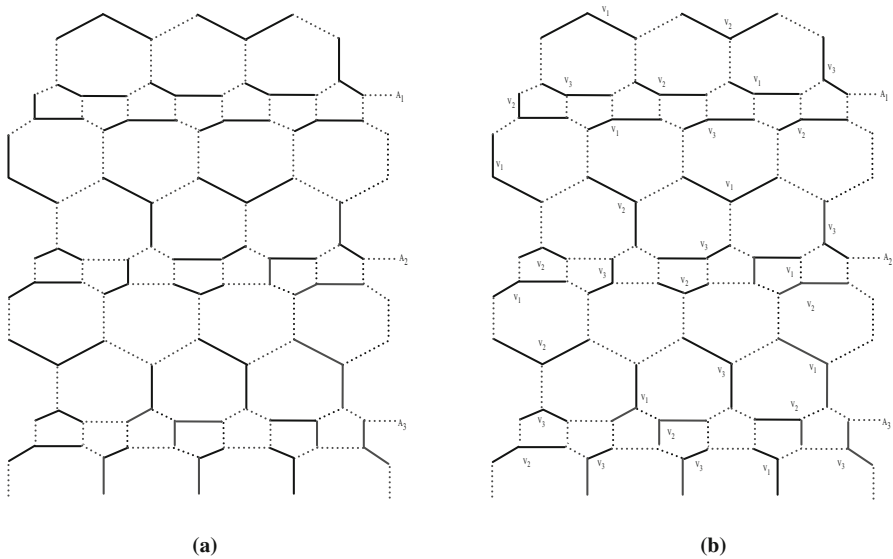


Fig. 9 **a** Induced P_3 -packing of $HAC_5C_7[4, 3]$, **b** Induced P_3 -packing 3 - partition for $HAC_5C_7[4, 3]$

9 $HAC_5C_7[n, m]$ carbon nanotube

A C_5C_7 net is a trivalent decoration made by alternating C_5 and C_7 . In $HAC_5C_7[n, m]$, the three first rows of vertices and edges are repeated alternatively. In each phase there are $8n$ vertices and n vertices which are joined to the end of the graph and hence the number of vertices in this nanotube is equal to $8nm + n$ [15]. In this section we compute the perfect P_3 -packing and an induced P_3 -packing k -partition number for $HAC_5C_7[n, m]$ nanotube. In $HAC_5C_7[n, m]$ nanotube, n denotes number of heptagons in one row and m denotes the number of repetition of the first three rows of vertices and edges.

In view of Theorem 2.1 we have the following result.

Theorem 9.1 *Let G be a $HAC_5C_7[n, m]$ nanotube and $H \simeq P_3$, then $\lambda(G, P_3) \leq \left\lfloor \frac{8nm + n}{3} \right\rfloor$.*

Lemma 9.2 *Let $G \simeq HAC_5C_7[4, k+1]$, $k \geq 1$, $H \simeq P_3$. Then $\lambda(G, H) = 11(k+1)$.*

Proof We prove the result by induction on k . When $k = 1$, $\lambda(G, H) = 22$. See Fig. 9. Assume that $\lambda(HAC_5C_7[4, k-1], H) = 11(k-1)$. Now $HAC_5C_7[4, k+1]$ is obtained by adding two phases $C_5 C_7$ to $HAC_5C_7[4, k-1]$ that induce the path P_3 . Thus $\lambda(HAC_5C_7[4, k+1], P_3) = \lambda(HAC_5C_7[4, k-1], P_3) + 2 = 11(k-1) + 2 = 11(k+1)$.

We proceed to prove that $\lambda(HAC_5C_7[n, m], P_3) = \left\lfloor \frac{(8nm + n)}{3} \right\rfloor$. Let the subgraph induced by the vertices of rows i and $i+1$ be denoted by A_i , $1 \leq i \leq n$.

Procedure Packing $(HAC_5C_7[n, m], P_3)$:

Input: The nanotube ($HAC_5C_7[n, m]$) and $H \simeq P_3$.

Algorithm:

- (i) Obtain a H -packing of A_1 as in Lemma 9.2. Then obtain a H -packing of A_2 by taking the mirror image of H -packing of A_1 , placing the mirror horizontal to the vertical, acute, obtuse edges from A_1 .
- (ii) Repeat step (i) for the subgraphs $A_i \cup A_{i+1} \cup A_{i+2} \cup \dots \cup A_n$, where $1 \leq i \leq n$.
- (iii) Obtain a H -packing of A_n as in A_1 when $n \equiv 0, 1, 2 \pmod{3}$.

Output: There exists perfect H -packing of nanotube $HAC_5C_7[n, m]$, with $\lfloor \frac{(8mn + n)}{3} \rfloor$ copies of H where $H \simeq P_3$.

Proof of correctness: In nanotube $HAC_5C_7[n, m]$, the induced subgraphs A_i , $1 \leq i \leq n$ are vertex disjoint. The algorithm covers all vertices of $HAC_5C_7[n, m]$, when $n \equiv 0 \pmod{3}$ and leaves one or two vertices unsaturated when $n \equiv 1, 2 \pmod{3}$. Thus $\lambda(G, H) = \lfloor \frac{(8mn + n)}{3} \rfloor$. \square

Lemma 9.3 The induced P_3 -packing k -partition number for $HAC_5C_7[n, m]$ nanotube is 3.

Proof Let G be a $HAC_5C_7[n, m]$ nanotube. We now give a procedure and its proof of correctness to show that $ipp(HAC_5C_6C_7[n, m], P_3) = 3$. \square

Procedure Partition for ($HAC_5C_7[n, m], P_3$)

Input: The induced P_3 -packing k -partition number for $HAC_5C_7[n, m]$ nanotube is 3.

Algorithm:

- (i) Choose a P_3 path on 3 vertices as in Fig. 9. The adjacent vertices of V_1 cannot be partitioned into V_2 alone. It fails the definition of induced P_3 -packing k -partition.
- (ii) Start a path of P_3 -packing of V_1 -partition. The adjacent path of partition of V_1 is either V_2 or V_3 .
- (iii) Start a path of P_3 -packing of V_2 -partition. The adjacent path of partition of V_2 is either V_3 or V_1 .
- (iv) Construct a path of P_3 -packing of V_3 -partition. The adjacent path of partition of V_3 is either V_2 or V_1 .
- (v) Continue the process of (ii), (iii) and (iv) where all the vertices are covered and partitioned into 3-partition.

Output: Induced P_3 -packing 3-partition number for $HAC_5C_7[n, m]$ nanotube is 3.

Proof of correctness: Repeating the process (v) implies, that there exists induced perfect P_3 -packing 3-partition for $HAC_5C_7[n, m]$ nanotube.

10 Summary and future work

In this paper we have computed perfect and almost perfect H -packing and an induced H -packing k -partition number for Armchair carbon nanotube $ACNT[n, m]$, Zig-Zag carbon nanotube $ZCNT[n, m]$, Zig-Zag Polyhex Carbon nanotube $TUHC_6[2m, n]$,

Boron triangular carbon nanotubes $BNT_t[n, m]$, $TUC_4C_8(S)$, $TUC_4C_8(R)$, $HAC_5C_6C_7[n, m]$ and $HAC_5C_7[n, m]$ where $H \simeq P_3$ and C_4 -packing for $TUC_4C_8(R)$. It is interesting to explore further results in future to compute H -packing and an induced H -packing k -partition number for other nanostructures and other chemical graphs.

References

1. R. Bar -Yehuda, M. Halldorsson, J. Naor, H. Shachnai, I. Shapira, Scheduling split intervals, in: Proc. Thirteenth Annu.ACM-SIAM Symp, On Discrete Algorithms, 732-741 (2002)
2. J.A. Bondy, U.S.R. Murty, *Graph theory with applications*, vol. 290 (Macmillan, London, 1976)
3. R. Bejar, B. Krishnamachari, C. Gomes, B. Selman Distributed constraint satisfaction in a wireless sensor tracking system, workshop on distributed constraint reasoning (Joint Conf. on Artificial Intelligence, Internat, 2001)
4. F.T. Boesch, J.F. Gimpel, Covering points of a digraph with point-disjoint paths and its application to code optimization. J ACM (JACM) **24**, 192–198 (1977)
5. Y.R. Chen, C. Weng, S.J. Sun, Electronic properties of zigzag and armchair carbon nanotubes under uniaxial strain. J Appl Phys **104**, 114310–114317 (2008)
6. M. Eliaasi, B. Taeri, Hyper-wiener index of zigzag polyhex nanotubes. ANZIAM J. **50**, 75–86 (2008)
7. A. Felzenbaum, Packing lines in a hypercube. Discret Math **117**, 107–112 (1993)
8. I. Gutman, J.W. Kennedy, L.V. Quintas, Perfect matchings in random hexagonal chain graphs. J Math Chem **6**, 377–383 (1991)
9. L. Hardesty, *Self-assembling computer chips* (MIT News Office, Cambridge, 2010)
10. P.J.F. Harris, *Carbon nanotube science: synthesis properties and applications* (Cambridge University Press, Cambridge, 2009)
11. P. Hell, D. Kirkpatrick, On the complexity of a generalized matching problem, in: Proc. Tenth ACM symp. on theory of computing, 309-318 (1978)
12. A. Hope, Component placement through graph partitioning in computer-aided printed-wiring-board design. Elect Lett **8**(4), 87–88 (1972)
13. L.J. Hubert, Some applications of graph theory to clustering. Psychometrika **39**, 283–309 (1974)
14. S. Iijima, Helical microtubules of graphitic carbon. Nature **354**, 56–58 (1991)
15. A. Iranmanesh, M. Zeraatkar, Computing Ga index of $HAC_5C_7[p, q]$ and $HAC_5C_6C_7[p, q]$ nanotubes. Optoelect Adv Mater—Rapid Commun **5**(7), 790–792 (2011)
16. J. Kind, T. Niessen, R. Mathar, Theory of maximum packing and related channel assignment strategies for cellular radio networks. Math Methods Oper Res **48**, 1–16 (1998)
17. J. Kunstmann, A. Quandt, Broad boron sheets and boron nanotubes: an ab initio study of structural, electronic and mechanical properties. Phys Rev B **74**, 354–362 (2006)
18. M.A. Malik, S. Hayat, M. Imran, On the anti-Kekulé number of nanotubes and nanocones. J Comput Theor Nanosci **12**, 3125–3129 (2015)
19. M. Munir, W. Nazeer, S. Rafique, A. Nizami, S. Kang, Some computational aspects of boron triangular nanotubes. Symmetry **9**, 6 (2017)
20. A.Al. Mutairi, B. Ali, P. Manuel, Packing in carbon nanotubes. J Comb Math Comb Comput **92**, 195–206 (2015)
21. A. Muthumalai, I. Rajasingh, A.S. Shanthi, Packing of hexagonal networks. J Comb Math Comb Comput **79**, 121–127 (2011)
22. M.F. Nadeem, S. Zafar, Z. Zahid, On topological properties of the line graphs of subdivision graphs of certain nanostructures. Appl. Math. Comput. **273**, 125–130 (2016)
23. S.M.J. Raja, A. Xavier, I. Rajasingh, Induced H-packing k-partition problem in interconnection networks. Int J Comput Math Comput Syst Theory **2**, 136–146 (2017)
24. S.M.J. Raja, A. Xavier, A.S. Shanthi, Anti-Kekule number of certain nanotube structures. Int J Pure Appl Math **101**(5), 655–665 (2015)
25. I. Rajasingh, A. Muthumalai, R. Bharati, A.S. Shanthi, Packing in honeycomb networks. J Math Chem **50**(5), 1200–1209 (2012)

26. H.M.A. Siddiqui, M. Imran, Computation of metric dimension and partition dimension of nanotubes. *J Comput Theor Nanosci* **12**, 199–203 (2015)
27. K. Shailaja, T. Sameena, S.P. Sethy, P. Patil, Md. O Ashraf, Carbon nano tube: a review. *Indian J Res Pharm Biotechnol* **1**, 2321–5674 (2013)
28. S. Theresal, A. Xavier, S.M.J. Raja, Induced H-packing k-partition problem in certain networks. *Int J Recent Technol Eng Repr Issue* **8**(3), 1003–1010 (2019)
29. A. Xavier, S. Theresal, S.M.J. Raja, Induced H-packing k-partition number for certain nanotubes and chemical graphs. *J Math Chem* **58**, 1177–1196 (2020)
30. A. Xavier, S. Theresal, S.M.J. Raja, Induced H-packing k-partition number for certain graphs. *Int J Comput Sci Eng* **7**(9), 91–95 (2019)

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.