# Packing in Carbon Nanotubes

Abdullah Al Mutairi, Bader Ali and Paul Manuel
Department of Information Science,
College of Computing Science and Engineering,
Kuwait University

**Abstract**

Structures realized by arrangements of regular hexagons in the plane are of interest in the chemistry of benzenoid hydrocarbons, where perfect matchings correspond to kekule structures which feature in the calculation of molecular energies associated with benzenoid hydrocarbon molecules. Mathematically, assembling in predictable patterns is equivalent to *packing* in graphs. An $H$-packing of a graph $G$ is a set of vertex disjoint subgraphs of $G$, each of which is isomorphic to a fixed graph $H$. If $H$ is the complete graph $K_2$, the maximum $H$-packing problem becomes the familiar maximum matching problem. In this paper we find a $H$-packing of armchair carbon nanotube with $H$ isomorphic to $P_4$, *1, 4-dimethyl cyclohexane* and $C_6$. Further we determine the $H$-packing of zigzag carbon nanotube with $H$ isomorphic to *1, 4-dimethyl cyclohexane.*

## 1 Introduction and Terminology

Carbon nanotubes are one of the most commonly mentioned building blocks of nanotechnology. The strength and the remarkable physical properties of these structures make them a very unique material with a whole range of promising applications. Carbon nanotubes based sensors have shown many benefits over their past counterparts [15] and are suitable candidates for wireless sensor nodes [21] which are used in many applications, ranging from military target tracking to industrial monitoring [18, 23].

Various surface nanotemplates that are naturally or artificially designed at the nanometre scale have been used to form periodic nanostructure arrays [5]. Molecules arranging themselves into predictable designs on silicon chips could lead to microprocessors with much smaller circuit elements. Mathematically, assembling in predictable patterns is equivalent to *packing*

JCMCC **92** (2015), pp. 195-206

in graphs. An $H$-packing of a graph $G$ is a set of vertex disjoint subgraphs of $G$, each of which is isomorphic to a fixed graph $H$. An $H$-packing in $G$ is called *perfect* if it covers all vertices of $G$. If $H$ is the complete graph $K_2$, the maximum $H$-packing problem becomes the familiar maximum matching problem.

Structures realized by arrangements of regular hexagons in the plane are of interest in the chemistry of benzenoid hydrocarbons, where perfect matchings correspond to kekule structures which feature in the calculation of molecular energies associated with benzenoid hydrocarbon molecules [11]. $H$-Packing, is of practical interest in the areas of scheduling [1], wireless sensor tracking [3], wiring-board design, code optimization [14] and many others. Packing lines in a hypercube has been studied in [9]. Algorithms are available for dense packing of trees of different sizes [24] and packing almost stars [8] into the complete graph. Further $H$-packing is determined for honeycomb [22] and hexagonal network [20]. In this paper we find a $H$-packing of armchair carbon nanotube with $H$ isomorphic to $P_4$, *1, 4-dimethyl cyclohexane* and $C_6$. Further we determine the $H$-packing of zigzag carbon nanotube with $H$ isomorphic to *1, 4-dimethyl cyclohexane.*

# 2 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 [6, 12, 17, 19] based on the rolling of $2D$ carbon hexagonal sheet. 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 $ACNT(n, m)$. We label the vertices of armchair carbon nanotube as in Figure 1 [18]. $ACNT(n, m)$ has $nm$ vertices, $\binom{m(3n-2)}{2}$ edges and has only odd number of rows and even number of columns. Manuel [18] proved that perfect matching exists for armchair carbon nanotube.

**Definition 2.1.** *[7] An $H$-packing of a graph $G$ is a set of vertex disjoint subgraphs of $G$, each of which is isomorphic to a fixed graph $H$. The maximum number of vertex disjoint copies of $H$ in $G$ is called the packing number and is denoted by $\lambda(G, H)$.*

Determining maximum $\lambda(G, H)$ is called the maximum $H$-packing problem in $G$. When $H$ is a connected graph with at least three vertices, Kirkpatrick and Hell proved that the maximum $H$-packing problem is $NP$-complete [14]. In the sequel let $C_n$ and $P_n$ denote a cycle and a path

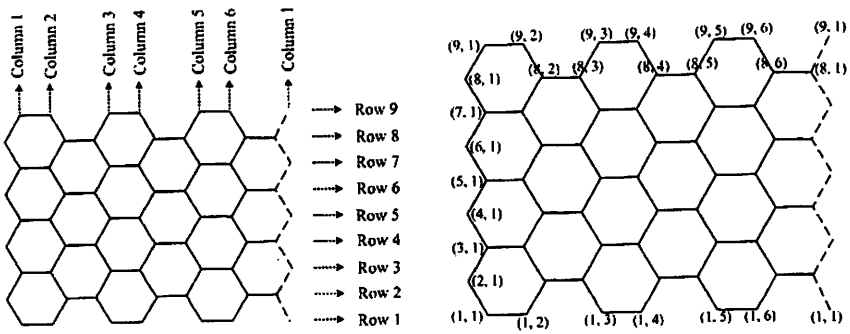


Figure 1: An armchair carbon nanotube

on $n$ vertices respectively. The vertices belonging to the subgraph $H$ of a $H$-packing are said to be saturated by the $H$-packing. The others are unsaturated. A perfect $H$-packing is a packing that saturates every vertex of $G$.

**Theorem 2.2.** *[22] Let $G$ be a graph and $H$ be a subgraph of $G$. Then* $\lambda(G,H) \leq \left\lfloor \frac{|V(G)|}{|V(H)|} \right\rfloor$.

### 2.0.1 Packing with $P_4$

In view of Theorem 2.2 we have the following result.

**Theorem 2.3.** *Let $G \simeq ACNT(n,m)$, and $H \simeq P_4$. Then* $\lambda(G,H) \leq \lfloor \frac{nm}{4} \rfloor$.

**Lemma 2.4.** *Let $G \simeq ACNT(2k+1,2)$, $k \geq 1$ and $H \simeq P_4$. Then* $\lambda(G,H) = \left\lfloor \frac{(2k+1)}{2} \right\rfloor$.

*Proof.* We prove the result by induction on $k$. When $k = 1$, $\lambda(G,H) = 1 = \lfloor \frac{3}{2} \rfloor$. See Figure 2 $(a)$. Assume that $\lambda(ACNT((2k-1,2),H) = \lfloor \frac{2k-1}{2} \rfloor$. Now $ACNT(2k+1,2)$ is obtained by adding a hexagon $C_6$ to $ACNT(2k-1,2)$ sharing the top two vertices of $ACNT(2k-1,2)$. The remaining vertices of $C_6$ induce path $P_4$. See Figure 2 $(b)$. Thus $\lambda(ACNT((2k+1,2),P_4) = \lambda(ACNT((2k-1,2),P_4) + 1 = \lfloor \frac{2k-1}{2} \rfloor + 1 = \lfloor \frac{2k+1}{2} \rfloor$.

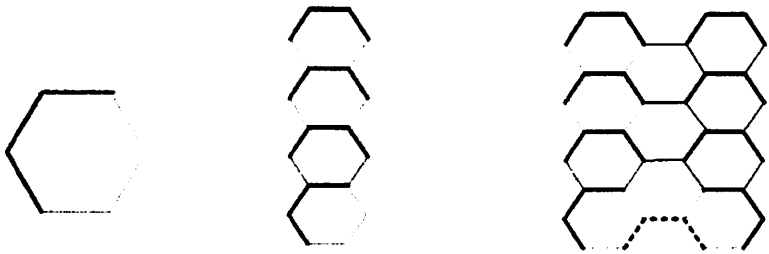


Figure 2: Dark lines show $P_4$-packing of $(a)$ $ACNT(3,2)$ $(b)$ $ACNT(9,2)$ $(c)$ $ACNT(9,4)$

We proceed to prove that $\lambda(ACNT((n,\ m),\ P_4) = \lfloor \frac{nm}{4} \rfloor$. 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** $(ACNT, P_4)$

**Input:** An armchair carbon nanotube $ACNT(n,m)$ and $H \simeq P_4$.

**Algorithm:**

(i) Obtain a $H$-packing of $A_1$ as in Lemma 2.4. Then obtain a $H$-packing of $A_3$ by taking the mirror image of the $H$-packing of $A_1$, placing the mirror perpendicular to the horizontal edges of $A_2$. Include the path induced by the vertices $(1,2)$, $(2,2)$, $(2,3)$ and $(1,3)$.

(ii) Repeat step (i) for the subgraphs $A_j \cup A_{j+1} \cup A_{j+2}$, $j = 4k-3$, $2 \leq k \leq \lfloor \frac{m}{4} \rfloor$.

(iii) Obtain a $H$-packing of $A_m$ as in $A_1$ when $m \equiv 2mod4$.

**Output:** There exists a perfect $H$-packing of $ACNT(n,m)$ with $\lfloor \frac{nm}{4} \rfloor$ copies of $H$ where $H \simeq P_4$.

**Proof of Correctness:** In $ACNT(n,m)$, the induced subgraphs $A_j$, $j$ odd, $1 \leq j \leq m$ are vertex disjoint. The algorithm covers all vertices of $ACNT(n,m)$ when $m \equiv 0mod4$ and leaves two vertices unsaturated when $m \equiv 2mod4$. Thus $\lambda(G,H) = \lfloor \frac{nm}{4} \rfloor$. □

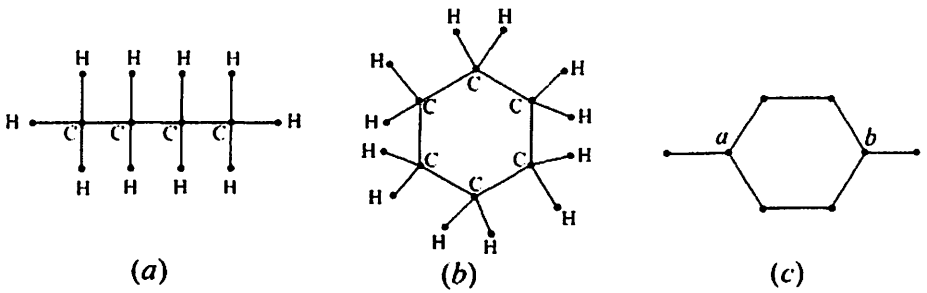


Figure 3: $(a)$ Butane $C_4H_{10}$ $(b)$ Cyclohexane $C_6H_{12}$ $(c)$ 1, 4-dimethyl cyclohexane

Chemists use diagrams to picture molecules, and these diagrams are also graphs. Usually the hydrogen atoms are omitted from the diagrams by the chemists using shorthand structure [13]. Figure 3 $(a)$ shows $C_4H_{10}$ butane structure and Figure 3 $(b)$ shows $C_6H_{12}$ cyclohexane structure. The removal of hydrogen atom leaves a path $P_4$ in the place of butane and $C_6$ in the place of cyclohexane.

### 2.0.2 Packing with *1, 4-dimethyl cyclohexane*

The neighborhood of a vertex $v$, $N(v)$, is $\{x \in V(G)/(x,v) \in E(G)\}$ and the closed neighborhood $N[v] = \{v\} \cup N(v)$. The graph in Figure 3 $(c)$ is known as *1, 4-dimethyl cyclohexane* in chemistry. Let $a$ and $b$ be the vertices of degree 3 as shown in Figure 3 $(c)$. We refer to $a$ and $b$ as a pair of opposite vertices.

**Theorem 2.5.** *Let $G \simeq ACNT(n,m)$ and $H \simeq$ 1, 4-dimethyl cyclohexane. Then $\lambda \leq \lfloor \frac{nm}{8} \rfloor - \lfloor \frac{m}{8} \rfloor$.*

*Proof.* We claim that in any $H$-packing of $ACNT(n,m)$ with $H \simeq$ *1, 4-dimethyl cyclohexane,* there are at least $\frac{m}{2}$ number of vertices in row 1 which remain unsaturated. There are at least $\lfloor \frac{3m}{8} \rfloor$ copies of $H$ induced by vertices in row 1, 2 and 3 consisting of $3m$ vertices. For $m \equiv 0 mod 4$, if $(1, j)$ and $(1, j+1)$, $j$ odd, $1 \leq j \leq m$ are saturated, then $(1, j-2)$, $(1, j-1)$, $(1, j+2)$, $(1, j+3)$ $jmodm$, $1 \leq j \leq m$ remain saturated. Therefore rows 1, 2 and 3 are packed by at most $\lfloor \frac{3m}{8} \rfloor - 1$ copies of $H$. This implies at least $\frac{m}{2}$ vertices of row 1 remain unsaturated. Similarly when, $m \equiv 2 mod 4$ there are at most $\lfloor \frac{3m}{8} \rfloor - 2$ copies of $H$ induced by rows 1, 2 and 3, which implies that at least $\frac{m}{2}$ vertices of row 1 are unsaturated. If the subgraph

$H$ is induced by vertices of rows 1, 2, 3, 4 and 5 then the five rows are packed by $\lfloor \frac{5m}{8} \rfloor$ copies of $H$. If vertex $(1, j)$, $1 \leq j \leq m$ is saturated then $(1, j-1)$ remains unsaturated. Therefore there are at most $\lfloor \frac{5m}{8} \rfloor - 1$ copies of $H$ if $m \equiv 0 mod 8$ and $\lfloor \frac{5m}{8} \rfloor$ copies of $H$ otherwise. In all cases in any $H$-packing, $\frac{m}{2}$ number of vertices remain unsaturated in row 1. In a similar manner $\frac{m}{2}$ number of vertices remain unsaturated in row $n$. Since $|V(H)| = 8$, we have $\lambda \leq \lfloor \frac{nm}{8} \rfloor - \lfloor \frac{m}{8} \rfloor$. □

**Procedure PACKING (*ACNT, 1, 4-dimethyl cyclohexane*)**

**Input:** An armchair carbon nanotube $ACNT(n, m)$, $n \equiv 1 mod 4$ and $H \simeq$ *1, 4-dimethyl cyclohexane.*

**Algorithm:**

Identify the vertex $a$ in $H$ with $(i, j)$, $i \equiv 2 mod 4$, $j$ odd, $1 \leq j \leq m$ and identify the corresponding vertex $b$ with $(i, j)$, $i \equiv 0 mod 4$, $j$ even, $1 \leq j \leq m$. See Figure 4 ($a$).

**End PACKING (*ACNT, 1, 4-dimethyl cyclohexane*)**

**Output:** A maximum $H$-packing of $ACNT$ with $H \simeq$ *1, 4-dimethyl cyclohexane* is $\lfloor \frac{nm}{8} \rfloor - \lfloor \frac{m}{8} \rfloor$.

**Proof of Correctness:** If $a$ and $b$ is a pair of opposite vertices, then the subgraph induced by $N[a] \cup N[b]$ is isomorphic to *1, 4-dimethyl cyclohexane.* Now $N[a] \cap N[b] = \Phi$ for all pairs of saturated vertices. Each row $i \equiv 2 mod 4$, $1 \leq i \leq n$ contains $\frac{m}{2}$ number of $a$'s in a *1, 4-dimethyl cyclohexane.* Hence $\lambda = \lfloor \frac{n}{4} \rfloor \times \frac{m}{2} = \lfloor \frac{nm}{8} \rfloor - \lfloor \frac{m}{8} \rfloor$. □

Thus we have the following result.

**Theorem 2.6.** *Let $G \simeq ACNT$, and $H \simeq$ 1, 4-dimethyl cyclohexane. Then $\lambda = \lfloor \frac{nm}{8} \rfloor - \lfloor \frac{m}{8} \rfloor$.*

### 2.0.3 Packing with $C_6$

Though armchair carbon nanotube is a $C_6$ tessellation, it is interesting to note that armchair carbon nanotube has perfect $H$-packing with $H \simeq C_6$ only when $n \equiv 0 mod 3$. In this section we give an algorithm for $H$-packing

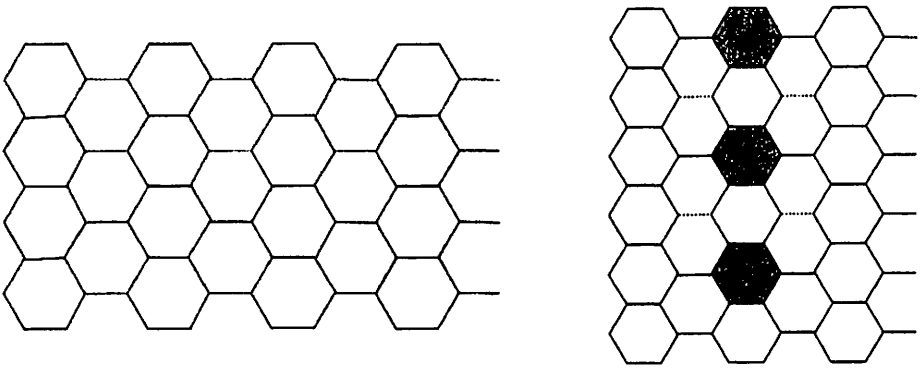

Figure 4: ($a$) $H$-packing of $ACNT(9,8)$ with $H \simeq 1$, 4-dimethyl cyclohexane ($b$) Shaded hexagons in $A_3$ are saturated

with $H \simeq C_6$ when $n \equiv 0 mod 3$ and improve the upper bound for all other cases. Further we prove that the upper bound obtained is sharp.

**Theorem 2.7.** *Let $G \simeq ACNT(n,m)$ and $H \simeq C_6$. Then $\lambda \leq \lfloor \frac{n}{3} \rfloor \times \frac{m}{2}$.*

*Proof.* Each $A_j$ is adjacent to $A_{j-1}$ and $A_{j+1}$, $1 \leq j \leq m$, $jmodm$ and each hexagons lies in three consecutive rows. If a hexagon is saturated in the row $i, i+1, i+2$ of $A_i$ then the hexagons in the row $i-1, i, i+1, i+2, i+3$ of $A_{i-1}$ and $A_{i+1}$ and the hexagons in the row $i+2, i+3, i+4, i-2, i-1$, $i$ of $A_i$ are unsaturated. Without loss of generality consider $A_1$, $A_2$, $A_3$ and $A_4$. Suppose alternate hexagons in $A_3$ are saturated then none of the hexagons in $A_2$ and $A_4$ are saturated. The saturated alternate hexagons leaves a row in between and the hexagons in that row of $A_2$ and $A_4$ are adjacent to saturated hexagon which cannot be saturated. See Figure 4 ($b$).

Suppose hexagons in a column are saturated in $A_3$ by skipping two columns of hexagons in between. In other words there are two unsaturated hexagons between two saturated hexagons. Then the hexagons adjacent to those two unsaturated hexagons in $A_2$ and $A_4$ are saturated. Thus the maximum number of hexagons saturated in each $A_j$ and $A_{j+1}$, $j$ odd, $1 \leq j \leq m$ is $\lfloor \frac{n}{3} \rfloor \times \frac{m}{2}$. □

**Procedure PACKING** $(ACNT, C_6)$

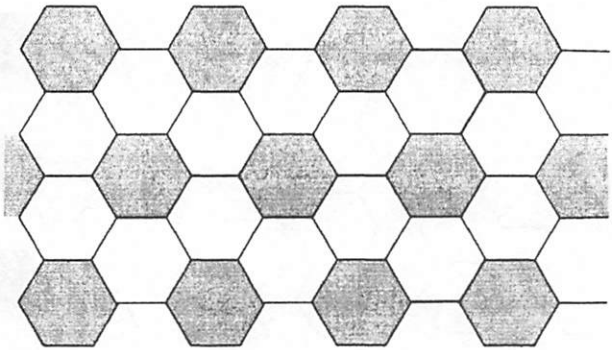

Figure 5: $H$-packing of $ACNT(9,8)$ with $H \simeq C_6$, shaded hexagons are saturated hexagon.

**Input:** An armchair carbon nanotube $ACNT(n,m)$ and $H \simeq C_6$.

**Algorithm:**

Saturate the hexagon induced by the vertices $(6i-5,j)$, $(6i-5,j+1)$, $(6i-4,j)$, $(6i-4,j+1)$, $(6i-3,j)$ and $(6i-3,j+1)$, $i = 1, 2, ...,$ $j$ odd $1 \leq j \leq m$ and also saturate the hexagon induced by the vertices $(6i-2,j)$, $(6i-2,j+1)$, $(6i-1,j)$, $(6i-1,j+1)$, $(6i,j)$ and $(6i,j+1)$, $i = 1, 2, ...,$ $j$ even $1 \leq j \leq m$, $jmodm$. See Figure 5.

**End PACKING** $(ACNT, C_6)$

**Output:** A perfect $H$-packing of $ACNT$ when $n \equiv 0mod3$ and a maximum $H$-packing of $ACNT$ otherwise.

**Proof of Correctness:** The hexagons saturated in the row $6i$, $6i-1$ and $6i-2$ are independent of the hexagons saturated in the row $6i-3$, $6i-4$ and $6i-5$. Further the number of hexagons in the rows induced by $i$, $i+1$ and $i+2$, $i = 1, 2, ...$ is $\frac{m}{2}$. Therefore $\lambda = \lfloor \frac{n}{3} \rfloor \times \frac{m}{2}$. □

**Theorem 2.8.** *Let $G \simeq ACNT(n,m)$, and $H \simeq C_6$. Then $\lambda = \frac{m}{2} \times \lfloor \frac{n}{3} \rfloor$.*

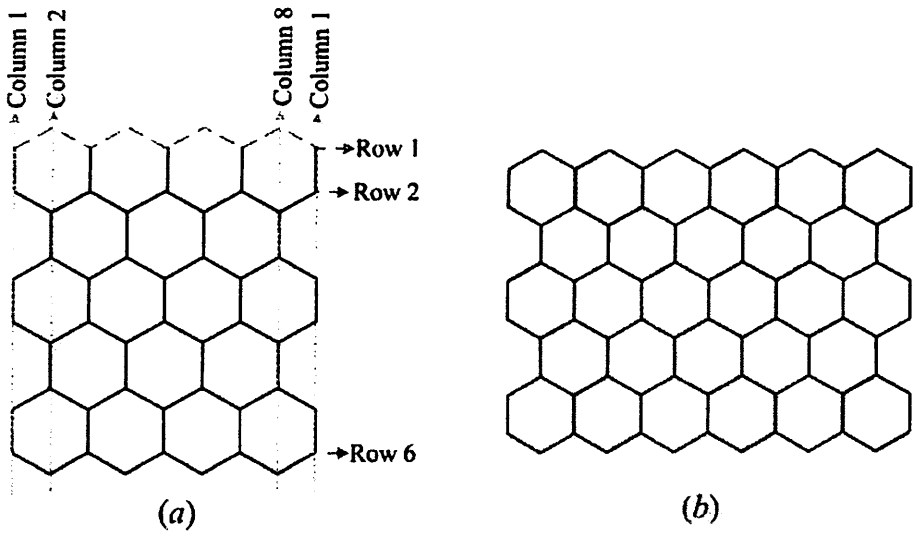


Figure 6: $(a)$ Zig-zag carbon nanotube $ZCNT(6,8)$ $(b)$ $H$-packing of $ZCNT(6,12)$ with $H \simeq$ 1, 4-dimethyl cyclohexane

# 3 Zig-Zag Carbon Nanotube

The Zig-zag carbon nanotube $ZCNT(n,m)$ has $n$ rows and $m$ columns is shown in Figure 6 $(a)$. The zig-zag carbon nanotube has only even number of rows and even number of columns and it has $nm$ vertices.

**Procedure PACKING** ($ZCNT(n,m)$, ***1, 4-dimethyl cyclohexane***)

**Input:** A zig-zag carbon nanotube $ZCNT(n,m)$, $m \equiv 0 mod 4$ and $H \simeq$ *1, 4-dimethyl cyclohexane.*

**Algorithm:** Identify the vertex $a$ in $H$ with $(i, 4j-3)$, $i$ even, $1 \leq i \leq n$, $1 \leq j \leq \lfloor \frac{m}{4} \rfloor$ and identify the corresponding vertex $b$ with $(i, 4j-1)$, $i$ odd, $1 \leq i \leq n$, $1 \leq j \leq \lfloor \frac{m}{4} \rfloor$. See Figure 6 $(b)$.

**End PACKING** ($ZCNT(n,m)$, ***1, 4-dimethyl cyclohexane***)

**Output:** A perfect $H$-packing of $ZCNT(n, m)$ when $m \equiv 0 mod 4$.

**Proof of Correctness:** Let $a$ and $b$ be a pair of opposite vertices. The subgraph induced by $N[a] \cup N[b]$ is isomorphic to *1, 4-dimethyl cyclohexane.* Further $N[u] \cap N[v] = \Phi$ for all pairs of saturated vertices. For $m \equiv 0 mod 4$, the subgraph induced by the vertices in rows $i$ and $i+1$, $i$ odd, $1 \leq i \leq n$ contains $\frac{m}{2}$ number of saturated vertices. The closed neighbourhoods of these saturated vertices together cover $8 \times \frac{m}{4} \times \frac{n}{2} = nm$ vertices. Therefore the $H$-packing is perfect and $\lambda = \lfloor \frac{nm}{8} \rfloor$. □

**Open Problem** Does there exists a perfect $H$-packing of $ZCNT(n, m)$ when $m \equiv 2 mod 4$ ?

# 4 Conclusion

In this paper we investigate various patterns embedded in the carbon nanotube. It would be interesting to consider packing in other nanotubes.

# References


[1] R. Bar-Yehuda, M. Halldorsson, J. Naor, H. Shachnai and I. Shapira, Scheduling split intervals, in: Proc. Thirteenth Annu.ACM–SIAM Symp. On Discrete Algorithms, (2002), 732–741.

[2] S. B. M. Bell, F. C. Holroyd and D. C. Mason, A digital geometry for hexagonal pixels, Image and Vision Computing, 7, (1989), 194-204.

[3] R. Bejar, B. Krishnamachari, C. Gomes and B. Selman, Distributed constraint satisfaction in a wireless sensor tracking system, Workshop on Distributed Constraint Reasoning, Internat. Joint Conf. on Artificial Intelligence, (2001).

[4] K. J. Burch, Chemical graph theory, Loci, (2008).

[5] W. Chen, A. T. S. Wee, Self-assembly on silicon carbide nanomesh templates, Journal of Physics D: Applied Physics, 40 (20), (2007).

[6] Y. R. Chen, C. Weng and S. J. Sun, Electronic properties of zigzag and armchair carbon nanotubes under uniaxial strain, Journal of Applied Physics, 104, (2008), 114310-114317.

[7] A. Czygrinow and M. Hanckowiak, Distibuted approximations for packing in unit-disk graphs, Distributed Computing: Proceedings of 21st International Symposium, Disc 2007, Lemesos, Cyprus, September 24-26, (2007).

[8] E. Dobson, Packing almost stars into the complete graph, Journal of Graph Theory, 10, (1997), 169-172.

[9] A. Felzenbaum, Packing lines in a hypercube, Discrete Mathematics 117, (1993), 107-112.

[10] G. Galli and D. Donadio, Thermoelectric materials: silicon stops heat in its tracks, Nature Nanotechnology 5, (2010), 701-702.

[11] I. Gutman, J. W. Kennedy and L. V. Quintas, Perfect matchings in random hexagonal chain graphs, Journal of Mathematical Chemistry, 6, (1991), 377-383.

[12] P. J. F. Harris, Carbon Nanotube Science: Synthesis, Properties and Applications; Cambridge University Press: Cambridge, UK, (2009).

[13] N. Hartsfield and G. Ringel, Pearls in graph theory, Dover Publications, INC Mineola, New York, (2003).

[14] P. Hell and D. Kirkpatrick, On the complexity of a generalized matching problem, in: Proc. Tenth ACM Symp. On Theory of Computing, (1978), 309–318.

[15] S. Joshi, R. Pathak and S. Ahmed, Wireless sensor network: intricate modeling and analysis of CNT and MEMS based sensor nodes, 2nd International Workshop on Electron Devices and Semiconductor Technology, (2009).

[16] A. K. Kelmans, Optimal packing of induced stars in a graph, Discrete Mathematics, 173, (1997), 97-127.

[17] J. Kunstmann and A. Quandt, Broad boron sheets and boron nanotubes: An ab initio study of structural, electronic, and mechanical properties, Phys. Rev. B, 74, (2006), 354-362.

[18] P. Manuel, Computational Aspects of Carbon and Boron Nanotubes, Molecules, 15, (2010), 8709-8722.

[19] P. Manuel and M. Guizani, Broadcasting algorithms of carbon nanotubes, Journal of Computational and Theoretical Nanoscience, 8, (2011), 1-9.

[20] A. Muthumalai, I. Rajasingh and A. S. Shanthi, Packing of Hexagonal Networks, Journal of Combinatorial Mathematics and Combinatorial Computation, 79, (2011), 121-127.

[21] R. Pathak and S. Joshi, Energy modeling in carbon nano tube based wireless sensor networks, First Asian Himalayas International Conference on Internet AH-ICI2009, (2009).

[22] I. Rajasingh, A. Muthumalai, R. Bharati and A. S. Shanthi, Packing in honeycomb networks, Journal of Mathematical Chemistry, 50 (5), (2012), 1200-1209.

[23] J. Sankman, H. Chen and D. Ma, Supercapacitor-based reconfigurable energy management unit for autonomous wireless sensor nodes, International Symposium on Circuits and Systems (ISCAS 2011), (2011), 2541-2544.

[24] H. P. Yap, Packing of graphs – A Survey, Discrete Mathematics 72, (1988), 395-404.