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ORIGINAL PAPER

Packing in honeycomb networks

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Abstract Molecules arranging themselves into predictable patterns on silicon chips could lead to microprocessors with much smaller circuit elements. 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 give algorithms to find a perfect packing of $HC(n)$ with P_6 and $K_{1,3}$ when n is even and thus determines their packing numbers. Further we also study the packing of $HC(n)$ with *1, 3-dimethyl cyclohexane*.

Keywords Matching · H-packing · F-packing · Perfect packing · Honeycomb networks

1 Introduction and terminology

Producing patterns with thin films of silicon to form nanomesh structures reduces their thermal conductivity without compromising their good electrical properties [7]. Further arranging molecules themselves into predictable patterns on silicon chips could lead to microprocessors with much smaller circuit elements [12]. The features on computer chips are getting so small that soon the process used to make them, which has hardly changed in the last 50 years, will not be applicable anymore. One of the

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alternatives that academic researchers have been exploring is to create tiny circuits using molecules that automatically arrange themselves into useful patterns. In a paper that appeared in "Nature Nanotechnology", MIT researchers have reported taking an important step towards this goal [9].

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. From the optimization point of view, maximum H-packing problem is to find the maximum number of vertex disjoint copies of H in G called the *packing number* denoted by $\lambda(G, H)$. For our convenience $\lambda(G, H)$ is sometimes represented as λ. 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 and feature in the calculation of molecular energies associated with benzenoid hydrocarbon molecules [8]. H-Packing, is of practical interest in the areas of scheduling [1], wireless sensor tracking [3], wiring-board design, code optimization [10] and many others.

An F-packing is a natural generalization of H-packing concept. For a given family F of graphs, the problem is to identify a set of vertex-disjoint subgraphs of G, each isomorphic to a member of F. The F-packing problem is to find an F-packing in a graph G that covers the maximum number of vertices of 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 [10]. Packing lines in a hypercube has been studied in [6]. Algorithms are available for dense packing of trees of different sizes [17] and packing almost stars [5] into the complete graph. In this paper we give algorithms to find a perfect packing of $HC(n)$ with P_6 and $K_{1,3}$ when n is even and thus determines their packing numbers. Further we also study the packing of $HC(n)$ with *1, 3-dimethyl cyclohexane*.

2 Honeycomb networks

Various surface nanotemplates that are naturally or artificially patterned at the nanometre scale have been used to form periodic nanostructure arrays. The formation mechanism of these nanomesh template is attributed to the self-assembly of accumulated carbon atoms into well-ordered honeycomb structures at the nanometre scale [4].

A honeycomb network can be built in various ways. The honeycomb network $HC(1)$ is a hexagon; see Fig. 1a. The honeycomb network $HC(2)$ is obtained by adding a layer of six hexagons to the boundary edges of $HC(1)$ as shown in Fig. 1b. Inductively honeycomb network $HC(n)$ is obtained from $HC(n-1)$ by adding a layer of hexagons around the boundary of $HC(n-1)$. The number of vertices and edges of $HC(n)$ are $6n^2$ and $9n^2-3n$ respectively [14]. If C_n^o denotes the outer cycle of $HC(n)$, then the number of vertices in C_n^o is $12n-6$. Let the top leftmost vertex in $HC(n)$ be denoted by x_n^o. See Fig. 1c.

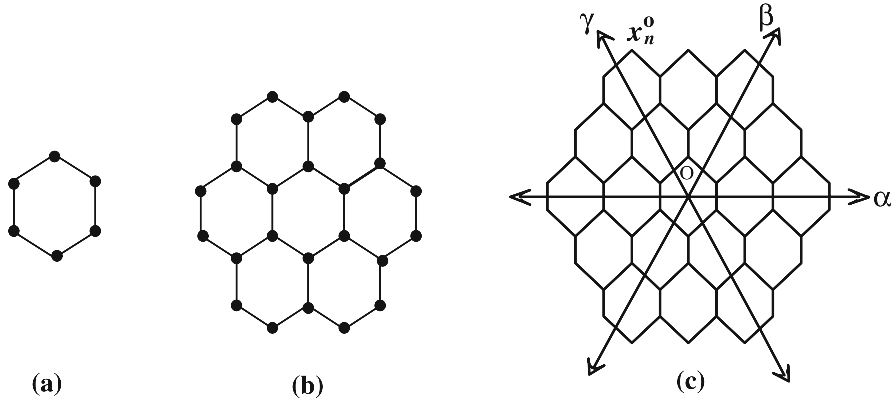


Fig. 1 **a** $HC(1)$ **b** $HC(2)$ **c** 3-dimensional honeycomb network

Honeycomb networks, thus built recursively using hexagonal tessellation, are widely used in computer graphics, cellular phone base station [15], image processing [2], and in chemistry as the representation of benzenoid hydrocarbons [14]. Honeycomb networks bear resemblance to atomic or molecular lattice structures of chemical compounds. In the sequel let C_n and P_n denote a cycle and a path on n vertices respectively. To prove the result in this paper we require to introduce co-ordinate axes for the honeycomb networks as follows:

The edges of $HC(1)$ are in 3 different directions. If the perpendicular bisectors of these edges meet at point O, then O is called the centre of the honeycomb network $HC(1)$. O is also considered to be the center of $HC(n)$. Through O draw three lines perpendicular to the three edge directions and name them as α, β, γ axes. See Fig. 1c. The α line through O, denoted by α_0, passes through $2n-1$ hexagons. Any line parallel to α_0 and passing through $2n-1-i$ hexagons is denoted by α_i, $1 \le i \le n-1$ if the hexagons are in the clockwise sense about α_o and by α_{-i}, $1 \le i \le n-1$ if the hexagons are in the anti-clockwise sense about α_0. In the same way $\beta_j, \beta_{-j}, 0 \le j \le n-1$, and $\gamma_k, \gamma_{-k}, 0 \le k \le n-1$ are defined.

3 A tight upper bound for $\lambda(G, H)$

In this section, we obtain an upper bound for $\lambda(G, H)$ and prove that the bound is tight.

Theorem 1 *Let G be a graph and H be a subgraph of G. Then* $\lambda(G, H) \le \left\lfloor \frac{|V(G)|}{|V(H)|} \right\rfloor$.

Proof It is clear that λ number of vertex disjoint copies of H in G cover $\lambda(G, H) \times |V(H)|$ distinct vertices of G. Therefore $\lambda(G, H) \times |V(H)| \le |V(G)|$. □

The following result is an easy consequence of the fact that $HC(n)$ has $6n^2$ vertices.

Theorem 2 *There exists a perfect H-packing of HC(n) with* n^2 *copies of H where* $H \simeq P_6$.

Proof By Theorem 1, $\lambda \leq n^2$. For $k = 1, 2, \ldots, n$ we have $C_k^o \simeq C_{12k-6}$. Let $V(C_k^o) = \{1, 2, \ldots, 12k-6\}$. Then $S_t = \{6t+1, 6t+2, 6t+3, 6t+4, 6t+5, 6t+6\}$ where $0 \leq t \leq 2k-2$ is a partition of C_k^o into paths of length 6. Therefore $\lambda \geq 1 + 3 + \cdots + (2n-1) = n^2$. Thus $\lambda = n^2$. □

Remark 1 If a graph G is perfectly packed by P_n then G is also perfectly packed by P_d for all divisors d of n.

In the view of Remark 1 it follows that $HC(n)$ can also be packed by P_2 and P_3. We further observe that $HC(n)$ can be packed by P_4 when n is even.

Conjecture *Let H be isomorphic to the graph $K_{1,3}$ with one edge replaced by a path of length 3. Then there exists a perfect H-packing of $HC(n)$.*

4 Packing of $HC(n)$ with C_6

Though $HC(n)$ is a C_6 tessellation, it is interesting to note that $HC(n)$ does not have a perfect H-packing when $H \simeq C_6$. We begin this section with an algorithm to pack $HC(n)$ with C_6 and obtain a lower bound for λ (HC(n), C_6).

Procedure PACKING(HC(n), C_6)

Input: A honeycomb network G of dimension n and $H \simeq C_6$.

Algorithm:

(i) Select the hexagon $H = HC(1)$ isomorphic to C_6.
(ii) Having selected hexagon H, select the hexagons among the six hexagons (if they exist) each containing a vertex adjacent to a vertex in H which have not been already selected. $H \leftarrow H \cup \{selected\ hexagons\}$.
(iii) Repeat (ii) till it is not possible to select any more hexagons in G. See Fig. 2.

End PACKING

Output: An H-packing of G with $n^2 - n - 1$ copies of C_6 when $n \equiv 2\ (mod\ 3)$, and with $n^2 - n + 1$ copies of C_6 when $n \equiv 0, 1\ (mod\ 3)$.

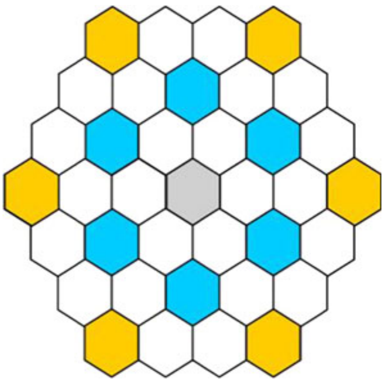


Fig. 2 Hexagons colored in $HC(4)$ are selected through PACKING $(HC(n), C_6)$

Proof of Correctness The selection process in (ii) implies that between any two selected hexagons through which an α-line passes, there are two adjacent hexagons which are not selected.

We observe that α_i, i even, passes through odd number of hexagons. By (i), $HC(1)$ has already been selected. Hence all middle hexagons through which the lines α_i, i even, pass are selected and every third hexagon along the same α-line from the already selected hexagons contribute to the set of selected hexagons. In otherwords, there are $2 \times \left\lfloor \frac{2n-i-2}{6} \right\rfloor + 1$ number of selected hexagons through which α_i, i even, passes.

For i odd, α_i passes through an even number of hexagons and the two adjacent middle hexagons remain not selected. The hexagons on either side of these two middle hexagons through which α_i passes are selected and every third hexagon is selected as in the case of α_i, i even. In otherwords, there are $2 \times \left\lceil \frac{2n-i-3}{6} \right\rceil$ number of selected hexagons through which α_i, i odd, passes.

Therefore,

$$\lambda \geq \begin{cases} 2\left[\sum_{i=2,4}^{n-1}\left(2\left\{\left\lfloor \frac{2n-i-2}{6}\right\rfloor\right\}+1\right)+\sum_{i=1,3}^{n-2} 2\left\lceil \frac{2n-i-3}{6}\right\rceil\right]+2\times\left\lfloor \frac{2n-2}{6}\right\rfloor+1 & n \text{ odd} \\ 2\left[\sum_{i=2,4}^{n-2}\left(2\left\{\left\lfloor \frac{2n-i-2}{6}\right\rfloor\right\}+1\right)+\sum_{i=1,3}^{n-1} 2\left\lceil \frac{2n-i-3}{6}\right\rceil\right]+2\times\left\lfloor \frac{2n-2}{6}\right\rfloor+1 & n \text{ even} \end{cases} \tag{1}$$

Let $n \equiv 2\ (mod\ 3)$. We begin with the case when n is even. Suppose $n = 6k + 2$, $k = 1, 2, 3, \ldots$. Then by (1) the number of selected hexagons is $2\left[9k^2 - k + 6k + 9k^2 + 5k\right] + 2 \times 2k + 1 = 36k^2 + 18k + 1 = n^2 - n - 1$.

On the otherhand when n is odd, let $n = 6k + 5$. $k = 1, 2, \ldots$. Again by (1), the number of selected hexagons is $n^2 - n - 1$. By a similar argument the result holds good when $n \equiv 0, 1\ (mod\ 3)$. □

Remark 2 The vertices of the selected hexagons are said to be saturated and all other vertices are unsaturated.

5 Honeycomb torus network

Honeycomb torus network can be obtained by joining pairs of nodes of degree two of the honeycomb network. In order to achieve edge and vertex symmetry, the best choice for wrapping around seems to be the pairs of nodes that are mirror symmetric with respect to three lines, passing through the center of the hexagonal network, and normal to each of the three edge orientations. Figure 3 shows how to wraparound honeycomb network of size three ($HC(3)$) to obtain $HT(3)$, the honeycomb torus of dimension three. The procedure PACKING ($HC(n)$, C_6) gives a lower bound for λ when $n \equiv 1, 2(mod\ 3)$. We prove that the lower bound is tight. The stratergy adopted is to find a perfect packing for the honeycomb torus and delete edges to obtain $HC(n)$ that contribute minimum number of selected hexagons.

Theorem 3 *For $n \equiv 1, 2(mod\ 3)$, there exists a perfect H-packing of $HT(n)$ where $H \simeq C_6$.*

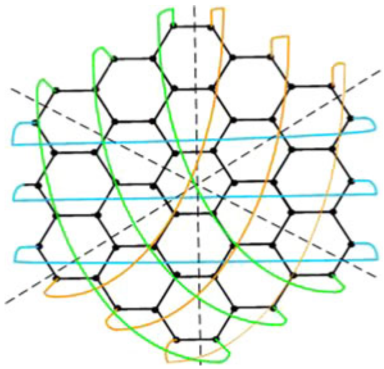


Fig. 3 Honeycomb torus of size three

Proof When $n \equiv 1\ (mod\ 3)$, the procedure PACKING $(HC(n), C_6)$ leaves $6(n-1)$ number of unsaturated vertices. On the otherhand, $n \equiv 2(mod\ 3)$ leaves $6(n+1)$ number of unsaturated vertices. The wraparound edges contribute $n-1$ or $n+1$ number of vertex disjoint cycles of length 6 which are also disjoint from the already chosen cycles obtained using Procedure PACKING $(HC(n), C_6)$, according as $n \equiv 1(mod\ 3)$ or $n \equiv 2(mod\ 3)$ respectively. Hence $\lambda = n^2$. □

Theorem 4 *Let* $G \simeq HC(n)$, $n \geq 3$ *and* $H \simeq C_6$. *Then* $\lambda = \begin{cases} n^2 - n + 1 & for\ n \equiv 1\ (mod\ 3) \\ n^2 - n - 1 & for\ n \equiv 2\ (mod\ 3) \end{cases}$.

Proof Deletion of wraparound edges in $HT(n)$ yields $HC(n)$, and the contribution to λ by the hexagons formed using the wraparound edges is minimum. □

Conjecture *Let* $G \simeq HC(n), n \geq 3$ *and* $H \simeq C_6$. *Then* $\lambda = n^2 - n + 1$ *for* $n \equiv 0\ (mod\ 3)$.

6 Packing $HC(n)$ with claw

One of the most widely studied packing is claw-packing [5]. A claw is another name for the complete bipartite graph $K_{1,3}$. A claw-free graph is a graph in which no induced subgraph is a claw.

The packing of induced stars in a graph has been studied in [13]. Las Vergnas proved that the $\{S_1, \ldots, S_k\}$-packing problem where $S_t \simeq K_{1,t}$ is polynomially solvable [16]. On the contrary, Hell and Kirkpatrick [11] proved that the packing problem when $F = \{S_i : i \in J\}$ is *NP*-complete whenever $J \subseteq N$ is not of the form $\{1, 2, \ldots, k\}$. In this section we study the packing of $HC(n)$ with S_3.

Definition 1 The subgraph induced by C_i^o and C_{i-1}^o in $HC(n)$ is called a Circular channel and is denoted by $CC(i)$ for $i = 3, 5, \ldots, n$ if n is odd and for $i = 2, 4, \ldots, n$ if n is even.

Figure 4 is the Circular channels in $HC(3)$ and $HC(4)$.

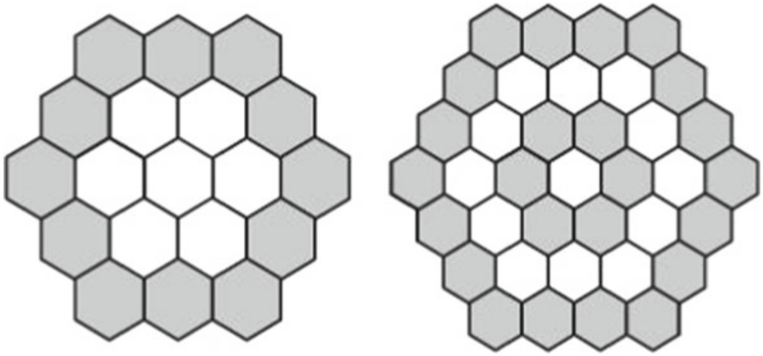


Fig. 4 Circular channels in $HC(3)$ and $HC(4)$

Definition 2 Given a vertex x in a hexagon, the unique vertex y at distance 3 from it is called the diagonally opposite vertex of x.

Procedure PACKING($HC(n)$, S_3)
Input: A honeycomb network G of dimension n and $H \simeq S_3$.
Algorithm:
Take $k = n$.
While $k \geq 2$ Do

(i) Start at a vertex u of degree 3 adjacent to x_n^o in $CC(k)$. Call u a saturated vertex. Saturate a sequence of diagonally opposite vertices of hexagons beginning with vertex u in the clockwise direction. Proceed till a vertex v of degree 2, if any, is reached. Fix the next vertex in the sequence as the vertex w at distance 3 from v on C_k^o. In addition saturate the unique vertex w' in $CC(k-2)$ at distance 4 from v.

(ii) Continue the process as in (i) beginning with w till vertex u is reached. See Fig. 5.

$k \leftarrow k - 2$.
Repeat
End PACKING
Output: A perfect H-packing of $HC(n)$ when n is even and an H-packing of $HC(n)$ with at most 18 unsaturated vertices, if n is odd.

Proof of Correctness The subgraph induced by $N[v]$ when v is a saturated vertex is isomorphic to S_3. Now $N[u] \cap N[v] = \Phi$ for all pairs of saturated vertices. For n even, $CC(k)$ contains $6(k-1)$ number of saturated vertices, $k = n, n-2, \ldots, 2$. The closed neighbourhoods of these saturated vertices together cover $4 \times 6[(n-1) + (n-3) + \cdots + 1] = 6n^2$ vertices. Therefore the H-packing is perfect and $\lambda = \left\lfloor \frac{6n^2}{4} \right\rfloor$.

For n odd, $CC(k)$ contains $6k - 9$ number of saturated vertices $k = n, n-2, \ldots, 3$ covering $4 \times 3\,[(2n-3) + (2n-7) + \cdots + 3] + 4 \times 3 \times \left(\frac{n-3}{2}\right) = 6n^2 - 18$ vertices. Therefore $\lambda \geq \left\lfloor \frac{6n^2}{4} \right\rfloor$. □

The graph in Fig. 6 is known as *1, 4-dimethyl cyclohexane* in chemistry.

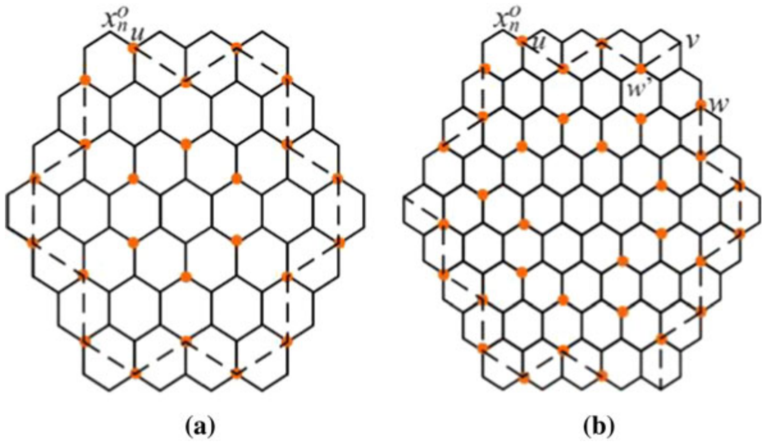
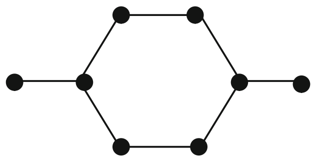


Fig. 5 H-packing of $HC(n)$ when $H \simeq S_3$ by traversing through diagonally opposite vertices of hexagons. **a** $HC(4)$, **b** $HC(5)$

Fig. 6 1, 4-dimethyl cyclohexane



Corollary 1 *When H is isomorphic to 1, 4-dimethyl cyclohexane, there exists a perfect H-packing of HC(n) when n is even.*

Proof It is clear that the vertex set of each selected H obtained from PACKING $(HC(n), S_3)$ can be partitioned into two disjoint sets each inducing a subgraph isomorphic to S_3. □

The algorithm PACKING $(HC(n), S_3)$ leaves 18 unsaturated vertices in $HC(n)$ when n is odd. With the introduction of F-packing we modify the algorithm to pack $HC(n)$ with an F-packing where $F = \{S_3, S_2\}$ with maximum number of copies of S_3, and the rest being S_2.

Procedure PACKING(HC(n), {S_3, S_2})

Input: A honeycomb network G of dimension n, n odd, and $F = \{S_3, S_2\}$.

Algorithm:

(i) Call Procedure PACKING $(HC(n), S_3)$.

(ii) The 18 unsaturated vertices excluded in the algorithm induce three paths each of length 2 with 3 of the corner vertices as the center vertices of these paths together with three more paths each of length 2 with three independent vertices of $HC(1)$ as center vertices.

End PACKING

Output: An F-packing of $HC(n)$ with $\left\lfloor \frac{6n^2}{4} \right\rfloor - 4$ copies of S_3 and six copies of S_2.

Proof of Correctness The copies of S_3 and S_2 selected by the procedure are disjoint and cover $4 \times \left(\left\lfloor \frac{6n^2}{4} \right\rfloor - 4\right) + 6 \times 3 = 6n^2$ vertices. □

7 Packing *HC (n)* with 1, 3-dimethyl cyclohexane

The graph H in Fig. 7 is the well known structure in chemistry, known as *1, 3-dimethyl cyclohexane*. We call vertex u the top vertex of H, v the bottom vertex of H and t_1 and t_2 the tail vertices of H respectively. In this section we study the H-packing of $HC(n)$.

Procedure PACKING($HC(n)$, 1, 3-dimethyl cyclohexane)

Input: A honeycomb network G of dimension n and H isomorphic to a 1, 3-dimethyl cyclohexane.

Algorithm: Start at the top leftmost vertex x_n^o of $HC(n)$ as the top vertex of a 1, 3-dimethyl cyclohexane and identify H as a subgraph of $HC(n)$. Choose top vertices alternately in the hexagons through which the line α_i passes and the hexagons through which both α_i and α_{i-1} pass, $1 \le i \le n-1$. See Fig. 8.

Output: An H-packing of $HC(n)$ with $\lambda \ge \left\lfloor \frac{6n^2}{8} \right\rfloor - \left\lceil \frac{n}{2} \right\rceil$ when n is odd and $\lambda \ge \left\lfloor \frac{6n^2}{8} \right\rfloor - \left\lfloor \frac{n}{2} \right\rfloor$ when n is even.

Proof of Correctness The mirror images of the cycles selected in the Procedure PACKING ($HC(n)$, 1, 3-dimethyl cyclohexane) about the α_0 line together with the already

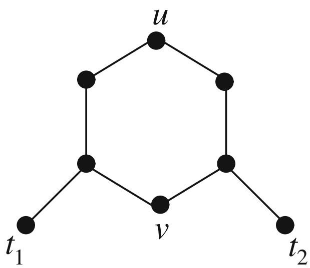


Fig. 7 1, 3-dimethyl cyclohexane

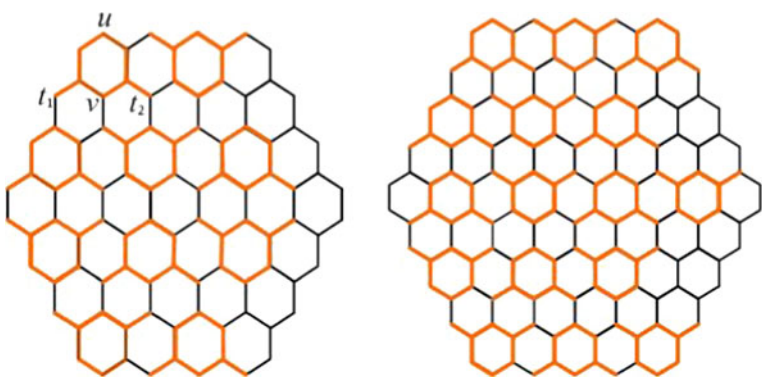


Fig. 8 Illustrating the procedure packing 1, 3-dimethyl cyclohexane in $HC(4)$ and $HC(5)$

selected ones yield a packing of 1, 3-dimethyl cyclohexane. We select 1, 3-dimethyl cyclohexane through which the lines $\alpha_{n-1}, \alpha_{n-3}, \ldots, \alpha_1$ pass when n is even. Hence $\lambda \geq 2[(n-1)+(n-2)+\cdots+\frac{n}{2}] = \left\lfloor \frac{6n^2}{8} \right\rfloor - \left\lfloor \frac{n}{2} \right\rfloor$.

We also select 1, 3-dimethyl cyclohexane through which the lines α_{n-1}, $\alpha_{n-3}, \ldots, \alpha_0$ pass when n is odd. Therefore $\lambda \geq (n-1)+2[(n-2)+(n-2)+(n-4)+(n-4)+\cdots+1+1] = \left\lfloor \frac{6n^2}{8} \right\rfloor - \left\lceil \frac{n}{2} \right\rceil$. □

8 Conclusion

In this paper we investigate various patterns embedded in the honeycomb network. This motivates us to consider packing in other benzenoid structures. As the study of packing is applicable to both chemistry and computer science, it would also be interesting to consider interconnection networks such as hexagonal mesh, butterfly networks, hypercube networks, benes networks, etc and find patterns that pack these networks.

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