

## DOMINATION, TOTAL DOMINATION AND OPEN PACKING OF THE CORCOR DOMAIN OF GRAPHENE

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**Abstract.** A dominating set of a graph  $G = (V, E)$  is a subset  $D$  of  $V$  such that every vertex not in  $D$  is adjacent to at least one vertex in  $D$ . A dominating set  $D$  is a total dominating set, if every vertex in  $V$  is adjacent to at least one vertex in  $D$ . The set  $P$  is said to be an open packing set if no two vertices of  $P$  have a common neighbor in  $G$ . In this paper, we obtain domination number, total domination number and open packing number of the molecular graph of a new type of graphene named CorCor that is a 2-dimensional carbon network.

**Keywords.** Graph; vertex; dominating set; domination number; total domination number.

### 1. Introduction

Throughout this paper, all graphs are assumed to be simple connected, undirected with  $n \geq 1$  vertices and  $m$  edges. Let  $G = (V, E)$  be a graph with the vertex set  $V = V(G)$  and the edge set  $E = E(G)$ . By the neighborhood of a vertex  $v$  of  $G$ , we mean the set  $N_G(v) = N(v) = \{u \in V : uv \in E\}$ . The closed neighborhood of vertex  $v$  is  $N_G[v] = N(v) \cup v$ . For  $S \subseteq V$ , the neighborhood of  $S$  is  $N(S) = \cup_{v \in S} N(v)$  and the closed neighborhood of  $S$  is  $N[S] = N(S) \cup S$ .

A set  $P$  of vertices of  $G$  is an open packing of  $G$ , if the open neighborhoods of the vertices of  $P$  are pairwise disjoint in  $G$ . The open packing number of  $G$ , denoted by  $\rho^0(G)$ , is the maximum cardinality among all open packings of  $G$ .

A subset  $D \subseteq V(G)$  is a dominating set of  $G$  if every vertex of  $V(G) - D$  has a neighbor in  $D$ . The domination number of  $G$ , denoted by  $\gamma(G)$ , is the minimum cardinality of a dominating set of  $G$ . A subset  $D \subseteq V(G)$  is a total dominating

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set, abbreviated TDS, of  $G$  if every vertex of  $G$  has a neighbor in  $D$ . The total domination number of  $G$ , denoted by  $\gamma_t(G)$  and introduced by Cockayne, Dawes, and Hedetniemi [2],[4].

Open packing is the natural dual object of total dominating sets, and so  $\rho^0(G) \leq \gamma_t(G)$  holds for every graph  $G$ , [5]. Moreover, if there exists a total dominating set  $D$  of  $G$  and  $D$  is also an open packing, then  $\rho^0(G) = \gamma_t(G) = |D|$ .

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  $H$ . 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  $\lambda$ . 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.  $H$ -Packing, is of practical interest in the areas of scheduling, wireless sensor tracking, wiring-board design, code optimization and many others. A benzenoid system is a geometric collection of congruent regular hexagons arranged in the plane, so that two hexagons are either disjoint or have a common edge. It follows from the conditions of regularity and congruence that benzenoid systems are subsets (with 1-connected interior) of a regular tiling of the plane by hexagonal tiles. Benzenoid systems are of considerable importance in theoretical chemistry because they are the natural graph representation of benzenoid hydrocarbons. In each benzenoid system as a graph, we assign vertices of hexagons as the vertices of the graph, and the sides of hexagons as the edges of the graph. Benzenoid graph is simple, plane, and bipartite. A vertex of a hexagonal system belongs to, atmost, three hexagons. A vertex shared by three hexagons is called an internal vertex, other vertices, it called external vertex.

Domination and its variations in graphs have attracted considerable attention, including a few chemically relevant applications, [6], [7] and [9]. A new 2-dimensional carbon network (benzenoid system), named Coronene of coronene (CorCor for short) was introduced by M. V. Diudea [3], [8]. CorCor is a benzene of benzenes, a domain of graphene. In this paper, we obtain domination number, total domination number and open packing number of the molecular graph of CorCor.

## 2. Domination Number of CorCor

In this paper we obtain domination number, total domination number and open packing for a new 2-dimensional carbon network, named CorCor.

The graphs  $G[n] = CorCor[n]$  with  $n$  layers (CorCor of dimension  $n$ ), have been shown in Figure 1. For  $n = 1$ , we have one coronene, for  $n = 2$ , this coronene is surrounded by 6 other coronenes, for  $n = 3$ , graph  $G[3]$  is obtained from  $G[2]$  surrounded by 12 coronenes and in general  $G[n]$  is obtained from  $G[n-1]$  surrounded by  $6(n-1)$  coronenes. Number of coronenes in  $G[n]$  are  $3n^2 - 3n + 1$ .

**Theorem 2.1.** ([7], Theorem 2.5) In a graph  $G$ , if there exists a perfect  $H$ -packing when  $H \cong K_{1,\Delta(G)}$ , then  $\gamma(G) = \lambda$ , where  $\Delta(G)$  and  $\lambda$  are the maximum degree and the packing number of  $G$  respectively.

By Theorem 2.1, packing number of CorCor[n] is equal with domination number because it is clear that  $\gamma(K_{1,\Delta(G)}) = 1$ . In a perfect  $H$ -packing when  $H \cong K_{1,\Delta(G)}$ , all the vertices are dominated by exactly one vertex. Hence, the packing number and the domination number of  $G$  are same. In other words  $\gamma(G[n]) = \lambda$ .

**Theorem 2.2.** Let  $G[n]$  be a CorCor of dimension  $n$ . Then

$$\gamma(G[n]) = \begin{cases} \frac{3}{2}(2n + \lceil \frac{n}{3} \rceil - 2)^2 + N - 34 & \text{if } \lceil \frac{n}{3} \rceil \text{ is even} \\ \frac{3}{2}(2n + \lceil \frac{n}{3} \rceil - 3)(2n + \lceil \frac{n}{3} \rceil - 1) + N - 34 & \text{if } \lceil \frac{n}{3} \rceil \text{ is odd} \end{cases}$$

where  $N = (n - \lceil \frac{n}{3} \rceil + 3)(n - \lceil \frac{n}{3} \rceil + 4)$ .

*Proof.* Let  $D$  be any minimum dominating set of  $G[n]$ . For computing  $\gamma(G[n])$ , it is enough to calculate  $|D|$ .

For  $n = 1$ , it is easy to see  $\gamma(G[1]) = 6$ . We determine vertices in dominating set  $G[2]$  and  $G[3]$  in Figure 3.2, also we can dominate  $G[3]$  with six hexagonal that it has been shown in Figure 3.2. The number of vertices of dominating set, respectively from interior of the hexagonal dominating to the outside as follows:

$$2, 6, 6, 12, 12, 18.$$

So  $\gamma(G[3]) = 2 + 6 + 6 + 12 + 12 + 18 + 24 = 80$ .

For  $n > 3$ , we have two cases.

**Case 1.** If  $\lceil \frac{n}{3} \rceil$  is even. Then the number of dominating vertices in a hexagonal dominating (see Figure 3.2,  $G[3]$ ) as follows:

$$2, 6, 6, 12, 12, \dots, 6(n-1), 6(n-1), 6n, 6(n - \lceil \frac{n}{3} \rceil + 3), 6(n - \lceil \frac{n}{3} \rceil + 2), \dots, 30.$$

Where:

$$\underbrace{2, 6, 6, 12, 12, \dots, 6(n-1), 6(n-1), 6n}_{(2n + \lceil \frac{n}{3} \rceil - 2)}$$

$$\underbrace{6(n - \lceil \frac{n}{3} \rceil + 3), 6(n - \lceil \frac{n}{3} \rceil + 2), \dots, 30}_{(n - \lceil \frac{n}{3} \rceil - 1)}$$

Also we have 24 vertices of dominating set are located out of hexagonal dominating. For obtaining  $\gamma(G[n])$ , it is that to sum the numbers.

**Case 2.** If  $\lceil \frac{n}{3} \rceil$  is odd. Then the number of dominating vertices in a hexagonal dominating (see Figure 3.2,  $G[3]$ ) as follows:

$$2, 6, 6, 12, 12, \dots, 6(n-1), 6(n-1), 6n, 6n, 6(n - \lceil \frac{n}{3} \rceil + 3), 6(n - \lceil \frac{n}{3} \rceil + 2), \dots, 30.$$

where

$$\underbrace{2, 6, 6, 12, 12, \dots, 6(n-1), 6(n-1), 6n, 6n}_{(2n + \lceil \frac{n}{3} \rceil - 2)}, \underbrace{6(n - \lceil \frac{n}{3} \rceil + 3), 6(n - \lceil \frac{n}{3} \rceil + 2), \dots, 30}_{(n - \lceil \frac{n}{3} \rceil - 1)}.$$

Similarly Case 1, we may to calculate the.  $\gamma(G[n])$ . The bold vertices in Figure 3.2 are in dominating set.  $\square$

**Theorem 2.3.** Let  $G[n]$  be a CorCor of dimension  $n$ . Then

$$\rho^0(G[n]) \geq 12n^2 - 12n + 4$$

This inequality is sharp.

*Proof.* We consider  $G$  be a CorCor of dimension  $n$ , we can see in Figure 3.3, number of vertices of open packing  $G[2]$  is shown,  $\rho^0(G[2]) = 29$ . As we mentioned earlier, number of coronenes in  $G[n]$  are  $3n^2 - 3n + 1$  and every coronenes can have four points from set of open packing, so

$$\rho^0(G[n]) \geq 4(3n^2 - 3n + 1)$$

Also  $\rho^0(G) \leq \gamma_t(G)$  holds for every graph  $G$ , according to the before theorem,  $\rho^0(G)$  have upper bound.

For  $n = 3$ , can see in Figure 3.3,  $\rho^0(G[3]) = 76$ , so inequality is sharp.  $\square$

In the next result the total domination of CorCor[n] is studied, but at first, we notice that the molecular graph of  $G[n]$  has exactly  $42n^2 - 24n + 6$  vertices and  $63n^2 - 45n + 12$  edges. The molecular graph  $G[n]$  is constructed from  $6n - 3$  rows of hexagons. For example, the graph  $G[3]$  has exactly 15 rows of hexagons and the number of hexagons in each row is according to the following sequence:

$$2, 5, 9, 10, 11, 12, 12, 11, 12, 12, 11, 10, 9, 5, 2.$$

The  $(3n - 1)^{th}$  row of  $G[n]$  is called the central row of  $G[n]$ . This row has exactly  $2(3\lceil \frac{n}{3} \rceil + 2(n - \lceil \frac{n}{3} \rceil)) - 3 = 4n + 2\lceil \frac{n}{3} \rceil - 3$  hexagons. The central hexagon of  $G[n]$  is surrounded by six hexagons. If we replace each hexagon by a vertex and

connect such vertices according to the adjacency of hexagons, then we will find a new hexagon containing the central hexagon of  $G[n]$  hexagon containing the last one and so on, see Figure 3.1. The hexagons constructed from this algorithm are called the big hexagons.

**Theorem 2.4.** Let  $G[n]$  be a CorCor of dimension  $n$ . Then

$$4(3n^2 - 3n + 1) < \gamma_t(G[n]) \leq \frac{|V(G[n])|}{3} + 6n - 2.$$

*Proof.* If  $G$  is a CorCor of dimension 1, then  $G[1]$  consists of just a single coronene, and it is easy to see that  $\gamma_t(G[1]) = 12$ . Now we consider the case of dimension at least two. In the CorCor, any zigzag line not containing vertical edges is called a zigzag horizontal line, [1]. The zigzag horizontal lines of CorCor are denoted by  $L_j, 1 \leq j \leq 6n - 2$ , Figure 3.4. We have

$$|L_1| = |L_{(6n-2)}|$$

and

$$\begin{aligned} L_1 &= \{v_{1,1}, v_{1,2}, v_{1,3}, v_{1,4}, v_{1,5}\}, \\ L_{(6n-2)} &= \{v_{(6n-2,1)}, v_{(6n-2,2)}, v_{(6n-2,3)}, v_{(6n-2,4)}, v_{(6n-2,5)}\}. \end{aligned}$$

Also

$$|L_2| = |L_{(6n-3)}|$$

And so on.

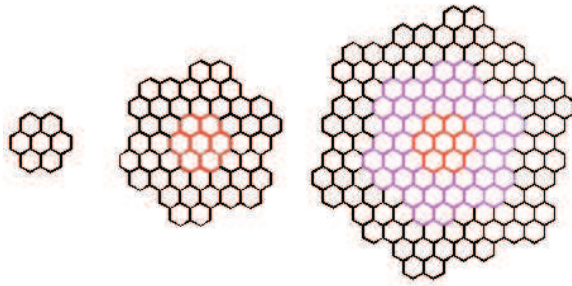
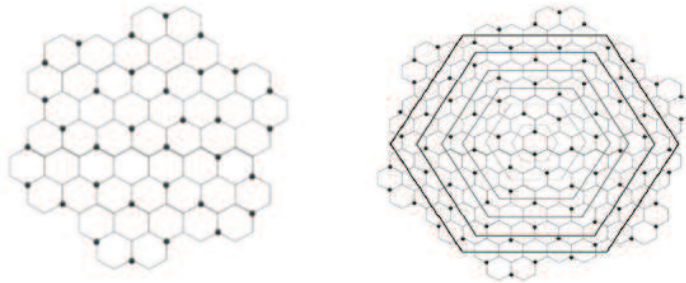
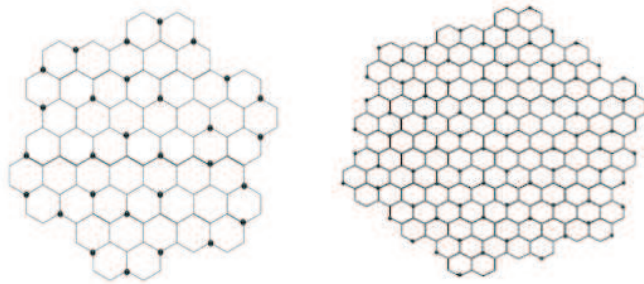
Let  $T$  be any minimum total dominating set of  $G[n]$ . For computing  $\gamma_t(G)$ , it is enough to calculate  $|T|$ .

$$\begin{aligned} |T| = 2|\{ &v_{1,3}, v_{1,4}, v_{2,1}, v_{2,2}, v_{2,7}, v_{2,8}, v_{2,9}, v_{3,1}, v_{3,2}, v_{3,7}, v_{3,8}, v_{3,13}, v_{3,14} \\ &, v_{4,2}, v_{4,5}, v_{4,6}, v_{4,11}, v_{4,12}, v_{4,15}, v_{5,2}, v_{5,3}, v_{5,8}, v_{5,9}, v_{5,14}, v_{5,15}, v_{6,4}\}|. \end{aligned}$$

Then  $|T| \leq \frac{|V(G[n])|}{3} + 6n - 2 = 14n^2 - 2n$ . Since  $\rho^0(G) \leq \gamma_t(G)$  holds for every graph  $G[5]$ . So that the inequality is hold. Also in Figure 3.5 is shown vertices of total dominating set of  $G[2]$ .  $\square$

### 3. Tables and Figures

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FIG. 3.1:  $G[n]=\text{CorCor}[n]$  for  $n=1,2,3$ .FIG. 3.2: Domination number of  $G[2]$  and Hexagonal dominating set of  $G[3]$ .FIG. 3.3: Open packing of  $G[2]$  and Open packing of  $G[3]$ .

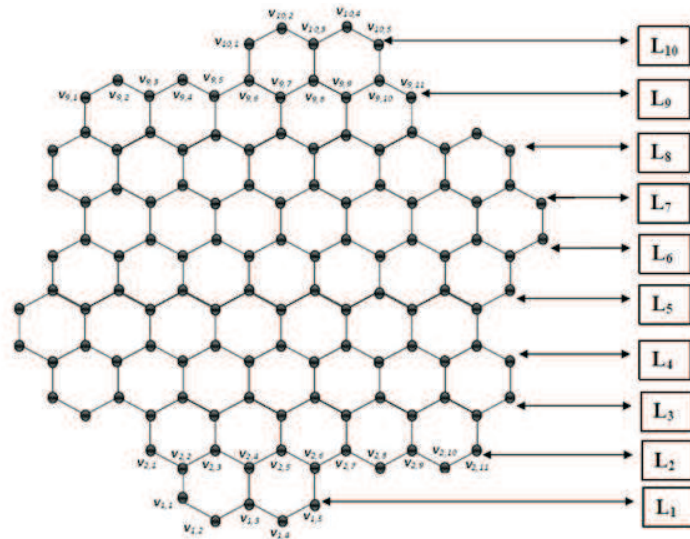


FIG. 3.4: The vertices and level in CorCor[2].

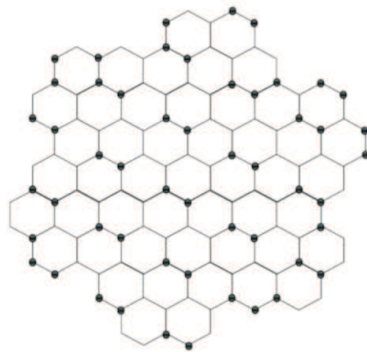


FIG. 3.5: Total domination number of CorCor[2].

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