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THE OMEGA POLYNOMIAL OF THE CORCOR DOMAIN OF GRAPHENE

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ABSTRACT. An opposite edge strip *ops* with respect to a given edge of a graph is the smallest subset of edges closed under taking opposite edges on faces. The Omega polynomial is a counting polynomial whose k-th coefficient is the number m(G,k) of *ops* containing k-edges. In this paper an exact formula for the Omega polynomial of the molecular graph of a new type of graphene named CorCor is given. As a consequence, the PI index of this nanostructure is computed.

Keywords: *Omega polynomial, CorCor*

INTRODUCTION

Throughout this paper, a graph means a simple connected graph. Suppose G is a graph and u, v are vertices of G. The distance d(u,v) is defined as the length of a shortest path connecting u and v in G. A graph can be described by a connection table, a sequence of numbers, a matrix, a polynomial or a derived unique number which is called a topological index. When we describe a graph by a polynomial as $P(G,x) = \Sigma_k m(G,k)x^k$, then we must find algorithms to compute the coefficients m(G,k), for each k, see [1-3].

Suppose G is a connected bipartite graph, with the vertex set V(G) and edge set E(G). Two edges e = uv and f = xy of G are called co-distant (briefly: e co f) if d(v,x) = d(v,y) + 1 = d(u,x) + 1 = d(u,y). It is far from true that the relation "co" is equivalence relation, but it is reflexive and symmetric.

Let $C(e) = \{ f \in E(G) \mid f \text{ co } e\}$ denote the set of edges in G, co-distant to the edge $e \in E(G)$. If relation "co" is an equivalence relation then G is called a co-graph. Consequently, C(e) is called an orthogonal cut *oc* of G and E(G) is the union of disjoint orthogonal cuts. If two consecutive edges of an edge-cut sequence are opposite, or "topologically parallel" within the same face/ring of the covering, such a sequence is called an opposite edge strip *ops* which is a quasi-orthogonal cut *qoc* strip. This means that the transitivity relation of the "co" relation is not necessarily obeyed. Any *oc* strip is an *op* strip but the reverse is not always true.

Let m(G,k) denote the multiplicity of a qoc strip of length k. For the sake of simplicity, we define m = m(G,k) and e = |E(G)|. A counting polynomial can be defined in simple bipartite graphs as $\Omega(G,x) = \Sigma_e m x^k$, named Omega

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polynomial of G. This polynomial was introduced by one of the present authors (MVD) [4]. Recently, some researchers computed the Omega and related polynomials for some types of nanostructures [5-10].

In this paper, we continue our earlier works on the problem of computing Omega polynomials of nanostructures. We focus on a new type of nanostructures named CorCor, a domain of the graphene – a 2-dimensional carbon network, consisting of a single layer of carbon atoms, and compute its Omega polynomial, Figure 1. Our notation is standard and mainly taken from the standard books of graph theory.

Main Results and Discussion

In this section, the Omega polynomial of G[n] = CorCor[n] with n layers (Figure 1) is computed. 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 $2\left(3\left\lceil \frac{n}{3}\right\rceil + 2(n - \left\lceil \frac{n}{3}\right\rceil)\right) - 3 = 4n + 2\left\lceil \frac{n}{3}\right\rceil - 3$ hexagons, where for a real number x, $\lceil x \rceil$ denotes the smallest integer greater or equal to x. 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]. Next consider the adjacency relationship between the hexagons of the second layer of G[n] and construct a new hexagon containing the last one and so on, see Figure 1. The hexagons constructed from this algorithm are called the big hexagons. By our algorithm, the hexagons of G[n] are partitioned into the following two classes of hexagons:

a) The hexagons crossing the edges of big hexagons, i.e. those depicted by thick line.
b) The hexagons outside the big hexagon.

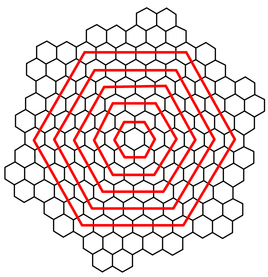

Figure 1. The Molecular Graph of CorCor[3].

One can see that the number of rows inside and outside big hexagons are equal to $\left(6\left\lceil \frac{n}{3} \right\rceil + 4(n - \left\lceil \frac{n}{3} \right\rceil)\right) - 4 = 4n + 2\left\lceil \frac{n}{3} \right\rceil - 4$ and $6n - 4 - (4n + 2\left\lceil \frac{n}{3} \right\rceil - 4) = 2n - 2\left\lceil \frac{n}{3} \right\rceil$, respectively. From Figure 1, one can see that the molecular graph of CorCor[n] can be partitioned into six equal parts with the same number of hexagons. If we consider one half of this graph then three cases of these six parts must be considered. Define three matrices A, A' and A'' as follows:

- A is an $\left(n - \left\lceil \frac{n}{3} \right\rceil\right) \times \left(2n - 2 + \left\lceil \frac{n}{3} \right\rceil\right)$ matrix with 0 & 1 entries. The entries corresponding to the hexagons of CorCor[n] are equal to 1, and other entries are zero, see Figure 2. As an example, the matrix A_6 is as follows:

$$A_6 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

- Suppose $A = [a_{ij}]$, $A' = [b_{ij}]$ is an $\left(2n - 2 + \left\lceil \frac{n}{3} \right\rceil\right) \times \left(n - \left\lceil \frac{n}{3} \right\rceil\right)$ matrix defined by

$$b_{ij} = \begin{cases} a_{\left(n - \left\lceil \frac{n}{3} \right\rceil - j + 1\right)(i + j - 1)} & i + j \le 2n - 1 + \left\lceil \frac{n}{3} \right\rceil \\ a_{\left(n - \left\lceil \frac{n}{3} \right\rceil - j + 1\right)\left(i + j - 2n + 1 - \left\lceil \frac{n}{3} \right\rceil\right)} & i + j > 2n - 1 + \left\lceil \frac{n}{3} \right\rceil \end{cases}$$

$A'' = [c_{ij}]$ is an $\left(2n - 2 + \left\lceil \frac{n}{3} \right\rceil\right) \times \left(n - \left\lceil \frac{n}{3} \right\rceil\right)$ matrix defined by $c_{ij} = a_{j\left(2n - 1 + \left\lceil \frac{n}{3} \right\rceil - i\right)}$.

It is easy to see that the number of hexagons in the central row of G[n] is $2\left(3\left\lceil \frac{n}{3} \right\rceil + 2\left(n - \left\lceil \frac{n}{3} \right\rceil\right)\right) - 3 = 4n + 2\left\lceil \frac{n}{3} \right\rceil - 3$. Suppose S'_i and S''_i denote the summation of all entries in the i[th] row of the matrices A' and A'', respectively. Then

$S'_i = \sum_{j=0}^{n-1-\lceil n/3 \rceil} a_{(n-j-\lceil n/3 \rceil)(i+j)}$ and $S''_i = \sum_{j=1}^{n-\lceil n/3 \rceil} a_{j(2n-i-1+\lceil n/3 \rceil)}$

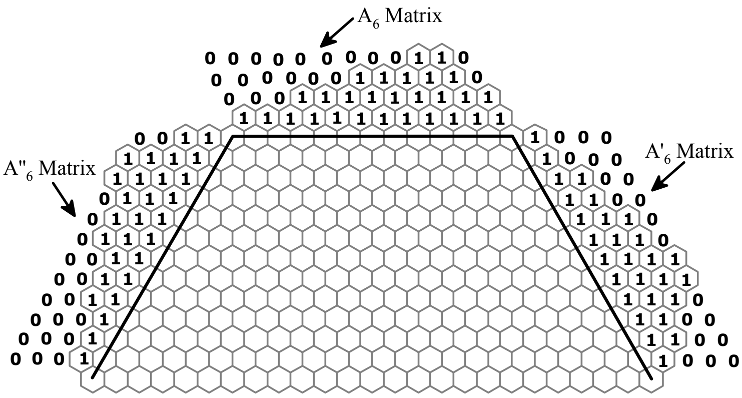

Figure 2. Construction of the Matrices A_6, A'_6 and A''_6.

and so,

$$\Omega(G[n],x) = 6\sum_{j=1}^{n-\lceil n/3\rceil} x^{3j-1+\lceil j/2\rceil}$$
$$+6\sum_{j=1}^{2n-2+\lceil n/3\rceil} x^{1+S'_j+S''_j+\left(2n+j-2+\lceil n/3\rceil\right)}$$
$$+3x^{4n-2+2\lceil n/3\rceil}$$

Thus for computing the omega polynomial of G[n], it is enough to compute S'_i and S''_i. By a simple calculations, one can see that Ω(G[1]) = $6x^3 + 3x^4$ and Ω(G[2]) = $6x^3 + 6x^6 + 15x^8$. So, we can assume that n ≥ 3. Our main proof consider three cases that n ≡ 0 (mod 3), n ≡ 1 (mod 3) and n ≡ 2 (mod 3).

We first assume that n ≡ 0 (mod 3). In this case the number of rows in the big hexagons is $7n/3 - 2$. By definition of A_n, if $1 \le j \le 4n/3 - 2$ then we have $S'_j = \lceil j/2\rceil$. If $4n/3 - 1 \le j \le 7n/3 - 2$ then we can define $j = 4n/3 - 2 + k$, where $1 \le k \le n$. Thus,

- $S'_i = 2n/3 - (2k-2)$, where k ≡ 1 or 2 (mod 3),
- $S'_i = 2n/3 - (2k-1)$, where k ≡ 0 (mod 3).

To compute S''_j, we consider four cases that $1 \le j \le n/3 - 1$, $j = n/3$, $j = n/3 + 1$ and $n/3 + 2 \le j \le 7n/3 - 2$. In the first case $S''_j = 2j$, and for the second and third cases we have $S''_j = 2n/3$. For the last case, we assume that j = n/3 + k + 1, 1 ≤ k ≤ 2n – 3. Then $S''_j = n - n/3 - \lceil k/3\rceil = 2n/3 - \lceil k/3\rceil$.
To compute the omega polynomial, we define the following polynomials:

1) $\varepsilon_1 = \sum_{j=1}^{n/3-1} x^{3j-1+7n/3+\lceil j/2\rceil}$,

2) $\varepsilon_2 = x^{-1+10n/3+\lceil n/6\rceil} + x^{1+10n/3+\lceil (n-3)/6\rceil}$,

3) $\varepsilon_3 = \sum_{j=n/3+2}^{4n/3-2} x^{3n-1+j+\lceil j/2\rceil-\lceil (3j-n-3)/9\rceil}$,

4) $\varepsilon_4 = \sum_{j=4n/3-1}^{7n/3-2} x^{j+7n/3+S'_j+S''_j}$.

Therefore, $\varepsilon_1+\varepsilon_2+\varepsilon_3+\varepsilon_4 = \sum_{j=1}^{2n-2+\lceil n/3\rceil} x^{1+S'_j+S''_j+(2n+j-2+\lceil n/3\rceil)}$.

To simplify these quantities, two cases that *n* is odd or even are considered. If *n* is even then

$$\Omega(G,x) = [6/(1-x^7)]\times\begin{pmatrix} x^3+x^6+x^{\frac{7n}{2}}\left(2x^1+x^4+x^5\right)- \\ x^{\frac{14n}{3}}\left(\frac{1}{2}x^{-2}+x^{-1}+2x^1+x^3+x^4+\frac{1}{2}x^5+\frac{n}{3}(-x^{-2}-2x^{-1}+x^5+2x^6)\right)\end{pmatrix}$$

if *n* is odd, then

$$\Omega(G,x) = [6/(1-x^7)]\times\begin{pmatrix} x^3+x^6+x^{\frac{7n}{2}}\left(x^{\frac{1}{2}}+x^{\frac{3}{2}}+2x^{\frac{9}{2}}\right)- \\ x^{\frac{14n}{3}}\left(\frac{1}{2}x^{-2}+x^{-1}+2x^1+x^3+x^4+\frac{1}{2}x^5+\frac{n}{3}(-x^{-2}-2x^{-1}+x^5+2x^6)\right)\end{pmatrix}$$

Using a similar argument as above, if $n \equiv 1$ (*mod 3*) then for even *n*,

$$\Omega(G,x) = [6/(1-x^7)]\times\begin{pmatrix} x^3+x^6+x^{\frac{7n}{2}}\left(2x+x^4+x^5\right)- \\ x^{\frac{14n}{3}}\left(\frac{2}{3}x^{\frac{-5}{3}}+\frac{5}{6}x^{\frac{-2}{3}}+x^{\frac{1}{3}}+x^{\frac{4}{3}}+2x^{\frac{10}{3}}+\frac{1}{3}x^{\frac{16}{3}}+\frac{1}{6}x^{\frac{19}{3}}+\frac{n}{3}(x^{\frac{19}{3}}+2x^{\frac{16}{3}}-2x^{\frac{-5}{3}}-x^{\frac{-2}{3}})\right)\end{pmatrix}$$

and for odd *n*,

$$\Omega(G,x) = [6/(1-x^7)]\times\begin{pmatrix} -x^3-x^6+x^{\frac{7n}{2}}\left(x^{\frac{1}{2}}+x^{\frac{3}{2}}+2x^{\frac{9}{2}}\right)- \\ x^{\frac{14n}{3}}\left(\frac{2}{3}x^{\frac{-5}{3}}+\frac{5}{6}x^{\frac{-2}{3}}+x^{\frac{1}{3}}+x^{\frac{4}{3}}+2x^{\frac{10}{3}}+\frac{1}{3}x^{\frac{16}{3}}+\frac{1}{6}x^{\frac{19}{3}}+\frac{n}{3}(-x^{\frac{19}{3}}-2x^{\frac{16}{3}}+2x^{\frac{-5}{3}}+x^{\frac{-2}{3}})\right)\end{pmatrix}$$

Finally, if $n \equiv 2$ (*mod 3*) then for even *n*,

$$\Omega(G,x) = [6/x^4(1-x^7)]\times\begin{pmatrix} x^7+x^{10}+x^{\frac{7n}{2}}\left(2x^5+x^8+x^9\right)- \\ x^{\frac{14n}{3}}\left(\frac{3}{2}x^{\frac{8}{3}}+x^{\frac{14}{3}}+x^{\frac{17}{3}}+x^{\frac{20}{3}}+x^{\frac{23}{3}}+\frac{1}{2}x^{\frac{29}{3}}+n(-x^{\frac{8}{3}}+x^{\frac{29}{3}})\right)\end{pmatrix},$$

and for odd *n*,

$$\Omega(G,x)=[6/x^4(1-x^7)]\times\left(\begin{array}{l} x^7+x^{10}+x^{\frac{7n}{2}}\left(x^{\frac{9}{2}}+x^{\frac{11}{2}}+2x^{\frac{17}{2}}\right)- \\ x^{\frac{14n}{3}}\left(\frac{3}{2}x^{\frac{8}{3}}+x^{\frac{14}{3}}+x^{\frac{17}{3}}+x^{\frac{20}{3}}+x^{\frac{23}{3}}+\frac{1}{2}x^{\frac{29}{3}}+n(-x^{\frac{8}{3}}+x^{\frac{29}{3}})\right)\end{array}\right)$$

It is now possible to simplify our calculations as follows:

$$\Omega(G,x)=[6/x^4(1-x^7)]\begin{cases} x^4\left(x^3+x^6+x^{7/2}(2x+x^4+x^5)-x^{14/3}\times R_0(x)\right) & n\equiv 0 \pmod 6\\ x^4\left(x^3+x^6+x^{7/2}(2x^{1/2}+x^{3/2}+2x^{9/2})-x^{14/3}\times R_1(x)\right) & n\equiv 1 \pmod 6\\ x^7+x^8+x^9+x^{10}+x^{12}-x^{14/3}\times R_2(x) & n\equiv 2 \pmod 6\\ x^4\left(x^3+x^6+x^{7/2}(2x^{1/2}+x^{3/2}+2x^{9/2})-x^{14/3}\times R_0(x)\right) & n\equiv 3 \pmod 6\\ x^4\left(x^3+x^6+x^{7/2}(2x+x^4+x^5)-x^{14/3}\times R_1(x)\right) & n\equiv 4 \pmod 6\\ x^7+2x^{17/2}+x^{10}+x^{23/2}+x^{25/2}-x^{14/3}\times R_2(x) & n\equiv 5 \pmod 6 \end{cases}$$

where,

$$R_0(x)=1/2x^{-2}+x^{-1}+2x+x^3+x^4+1/2x^5+n/3\left(-x^{-2}-2x^{-1}+x^5+2x^6\right),$$

$$R_1(x)=2/3x^{-5/3}+5/6x^{-2/3}+x^{1/3}+x^{4/3}+2x^{10/3}+1/3x^{16/3}+1/6x^{19/3},$$
$$+(n/3)\left(-2x^{-5/3}+x^{-2/3}+2x^{16/3}+x^{19/3}\right),$$

$$R_2(x)=(3/2-n)x^{8/3}+x^{14/3}+x^{17/3}+x^{20/3}+x^{23/3}+(n+1/2)x^{29/3}.$$

Since G[n] is a partial cube by a result of Klavzar [11],

$$\mathrm{PI(G[n])}=\mathrm{CI(G[n])}=\left[\Omega'(G[n],x)^2-\Omega'(G[n],x)-\Omega''(G[n],x)\right]_{x=1}$$

We now apply above calculations to compute the PI index of G[n]. We have:

$$\mathrm{PI(G[n])}=\begin{cases} 3969n^4-\frac{53333}{9}n^3+\frac{22769}{6}n^2-1196n+162 & n\equiv 0 \pmod 6\\ 3969n^4-\frac{53333}{9}n^3+\frac{22769}{6}n^2-1196n+\frac{2809}{18} & n\equiv 1 \pmod 6\\ 3969n^4-\frac{53333}{9}n^3+\frac{11458}{3}n^2-\frac{3743}{3}n+\frac{1504}{9} & n\equiv 2 \pmod 6\\ 3969n^4-\frac{53333}{9}n^3+\frac{22769}{6}n^2-1196n+\frac{321}{2} & n\equiv 3 \pmod 6\\ 3969n^4-\frac{53333}{9}n^3+\frac{22769}{6}n^2-1196n+\frac{1418}{9} & n\equiv 4 \pmod 6\\ 3969n^4-\frac{53333}{9}n^3+\frac{22769}{6}n^2-\frac{3584}{3}n+\frac{2837}{18} & n\equiv 5 \pmod 6 \end{cases}$$

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