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OMEGA POLYNOMIAL IN SUCOR NETWORK

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ABSTRACT. A new structurally functionalized graphene domain, called SuCor, was designed by combining the patterns of sumanene [6:(5,6)$_3$] and coronene [6:6$_6$]. The topology of the network is described in terms of Omega counting polynomial. Close formulas for calculating the polynomial and the Cluj-Ilmenau index derived from this polynomial are given.

Keywords: *sumanene, coronene, Sucor network, Omega polynomial*

INTRODUCTION

Several new carbon allotropes have been discovered and studied for applications in nano-technology, in the last twenty years, which can be assigned as the “Nano-era”. The impact of the Nano-Science resulted in reduction of dimensions of electronic devices and increasing their performances, al a lower cost of energy and money. Among the carbon new structures, fullerenes (zero-dimensional), nanotubes (one dimensional), graphene (two dimensional) and spongy carbon (three dimensional) are the most studied [1,2].

The present study deals with a hypothetical modified graphene, patterned by sumanene- and coronene-like units, of which topology is described in terms of Omega counting polynomial.

The lattice was built on the graphene sheet, of (6,3) tessellation, by decorating it with sumanene-like flowers, having coronene units as petals. The pattern, called Sucor, can be described as: {6:[5:(6:6$_6$)]$_3$}, with vertices/ atoms of degree 3 and 4, as shown in Figure 1 (below). This network is the twin of Corsu lattice {6:[6:(5,6)$_3$]$_6$}, also proposed by Diudea [3-5].

Notice, the coronene and sumanene are molecules synthesized in the labs [6-8]. Our idea about these networks was also supported by the synthesis of several bowl-shaped molecules, inspired from the architecture of fullerenes and, more recently, by the direct synthesis [9] of fullerenes starting from open precursors. The design and synthesis of various domains on the graphene sheet, eventually functionalized, is nowadays a challenge study and practice [10-13].

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OMEGA POLYNOMIAL

Let *G*(*V*,*E*) be a graph, with *V*(*G*) and *E*(*G*) being the set of vertices/ atoms and edges/bonds, respectively. Two edges *e* and *f* of a plane graph *G* are in relation *opposite, e op f,* if they are opposite edges of an inner face of *G*. Then *e co f* holds by the assumption that faces are isometric. The relation *co* is defined in the whole graph while *op* is defined only in faces/ rings (see below), thus being included in relation *co*. Relation *op* will partition the edges set of *G* into *opposite* edge *strips ops*, as follows. (i) Any two subsequent edges of an *ops* are in *op* relation; (ii) Any three subsequent edges of such a strip belong to adjacent faces; (iii) In a plane graph, the inner dual of an *ops* is a path, an open or a closed one (however, in 3D networks, the ring/face interchanging will provide *ops* which are no more paths); (iv) The *ops* is taken as maximum possible, irrespective of the starting edge.

The Ω-polynomial [14-17] is defined on the ground of opposite edge strips *ops* $S(G) = S_1, S_2, ..., S_k$ in the graph. Denoting by *m*, the number of *ops* of cardinality/length *s*=|*S*|, then we can write

$$\Omega(x) = \sum\nolimits_{s} m \cdot x^{s} \qquad (1)$$

The first derivative (in *x*=1) can be taken as a graph invariant or a topological index; in this case, it equals the number of edges in the graph.

$$\Omega'(1) = \sum\nolimits_{s} m \cdot s = e = \left|E(G)\right| \qquad (2)$$

We used here the topological description by Omega polynomial because this polynomial was created to describe the covering in polyhedral nanostructures and because is the best in describing the constitutive parts of nanostructures, particularly for large structures, with a minimal computational cost.

METHOD

In elaborating the close formula for counting the Omega polynomial, we followed the steps: (1) find the coefficients of x^1, .., x^6 in every Sucor unit; (2) find the number of common edges W_n between the Sucor units; (3) find the number of blue hexagons B_n (*i.e.*, triple joints); (4) find the coefficient of x^1, x^2,…,x^6 in the whole net; (5) find the formula to compute $\Omega(G,x)$ in a Sucor cyclic structure; (6) find W_n and B_n by a formula independent from common edges of the last complete cycle and (7) find a formula for $\Omega(G,x)$ in Sucor parallelogram structure.

Coefficients of x^1, …, x^6 in Sucor units

Local contributions to the polynomial coefficients are as follows.

The coefficient of $\mathbf{x^1}$ is equal to $(3\times6)+(2\times6)+(3\times2)=36$, for every Sucor unit.

The coefficients of $\mathbf{x^2}$ and $\mathbf{x^3}$ can be deduced from Figure 1, by following the red lines, in the left and right structures, respectively. In any 1/3 of Sucor units, there are 3 red lines, thus there are $3\times3=9$ red lines in each unit. Coefficient of $\mathbf{x^4}$ is derived as shown in Figure 2. The coefficient of x^5 is equal to 6 and the coefficient of x^6 is deduced from W_n and B_n (see Figure 2 and below).

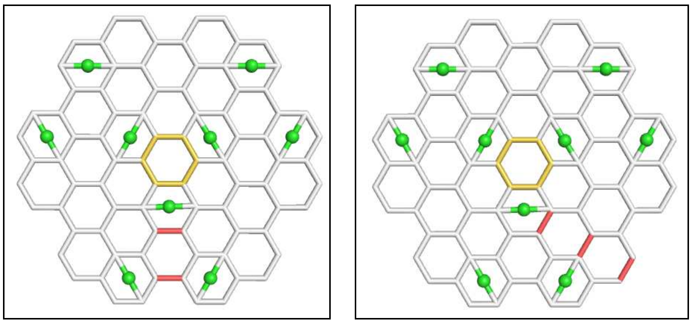

Figure 1. Ops of length 2 and 3 (edges marked in red).

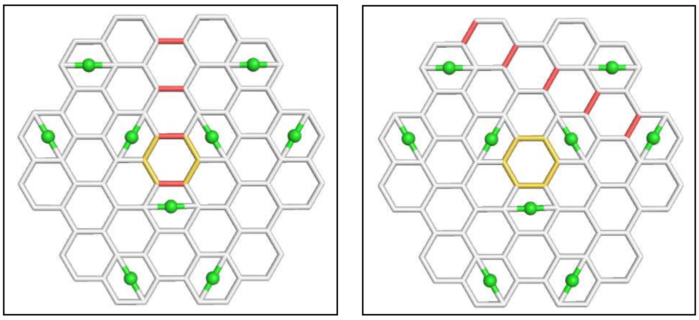

Figure 2. Ops of length 4 and 5 (edges marked in red).

Common edges (W_n) between Sucor units

"Common edges" means the edges common (i.e., double joints) of two SuCor units (Figure 3, in red). Clearly, $W_1=0$. Note, the colors have no chemical meaning (i.e., heteroatoms), they only help in describing the net. The center of SuCor units is yellow while the green points can be seen as bridges, in the chemical sense.

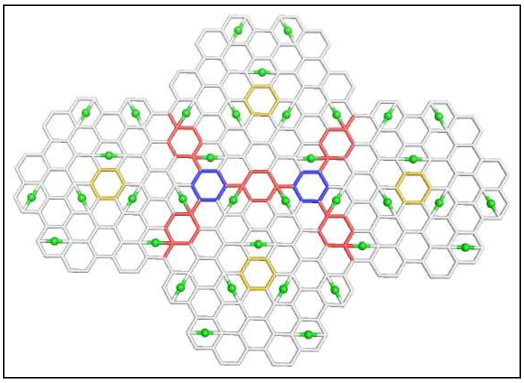

Figure 3. Network of four (*n*=4) Sucor units: yellow hexagons represent the unit core, while the blue one is the triple joints (B_n); the shared edges (W_n) between the units are marked in red.

We define r_k the number of Sucor units contained in a complete cyclic domain D_k, at the level *k*. For example $r_0=1$ and $r_1=7$, in general

$r_k = r_{k\text{-}1} + 6k$ or

$$r_k = 1 + 3k(k+1) \quad (3)$$

To compute W_n we must calculate the number of common edges of the last complete cyclic domain D_k and the number of common edges between the newly added units and the last complete cycle and the already added new units.

The addition of a unit is made stepwise around the complete cyclic domain D_k and results in either one common edge or two common edges. The number of units that make one common edge is $\left\lfloor \frac{n-r_{k-1}}{k} \right\rfloor$ while the number of units that make two common edges is $n-r_{k-1}-\left\lfloor \frac{n-r_{k-1}}{k} \right\rfloor$. So we have the following formula for W_n

$$W_n = W_{r_{k-1}} + \left\lfloor \frac{n-r_{k-1}}{k} \right\rfloor + 2\left(n-r_{k-1} - \left\lfloor \frac{n-r_{k-1}}{k} \right\rfloor \right) + (n-r_{k-1}-1) \quad (4)$$

For the special case when $n=r_k$, we need to add one more edge, thus we have:

$$W_n = W_{r_{k-1}} + \left\lfloor \frac{n-r_{k-1}}{k} \right\rfloor + 2\left(n-r_{k-1} - \left\lfloor \frac{n-r_{k-1}}{k} \right\rfloor \right) + (n-r_{k-1}) \quad (5)$$

Triple joint blue hexagons B_n

The triple joints denoted B_n are depicted in Figure 3 by blue hexagons that get join of three units. It is easily seen that B_1=B_2=0 and B_3=1 and B_4=2; in general, to compute B_n we can use the formula

$$B_n = B_{r_k - 1} + \left(n - r_{k-1} - \left\lfloor \frac{n - r_{k-1}}{k} \right\rfloor \right) + (n - r_{k-1} - 1) \tag{6}$$

When a cycle is completed, we have $n = r_k$ and one more edge must be added, thus:

$$B_n = B_{r_k - 1} + \left(n - r_{k-1} - \left\lfloor \frac{n - r_{k-1}}{k} \right\rfloor \right) + (n - r_{k-1} - 1) + 1 \tag{7}$$

Coefficients of x^1, x^2, …, x^6

For every complete cycle, the coefficient of $\mathbf{x^1}$ are:

$$6 \times 3 + 6 \times 2 + 3 \times 2 = 36.$$

This value is modulated by the contributions of double and triple joints, so the coefficient of **x** is $36n - 4W_n - 3B_n$. Every common edge reduces the value of coefficient of x^2 by 3, thus it will be $9n - 3W_n$. Next, every common edge will increase by 2 the coefficient of x^3, so that its value is $12n + 2W_n$. Similarly, we have: for x^4; $3n - W_n$; for x^5 ; $6n - 3B_n$; for x^6 ; $W_n + 3B_n$.

Omega polynomial in a Sucor cyclic structure

Now, we are able to write the formula for the Omega polynomial in case of a general cyclic Sucor structure (Figure 4, left):

$$\begin{aligned}\Omega(G,x) = {} & (36n - 4W_n - 3B_n)\, x + (9n - 3W_n)\, x^2 + (12n + 2W_n)\, x^3 \\ & + (3n - W_n)\, x^4 + (6n - 3B_n)\, x^5 + (W_n + 3B_n)\, x^6\end{aligned} \tag{8}$$

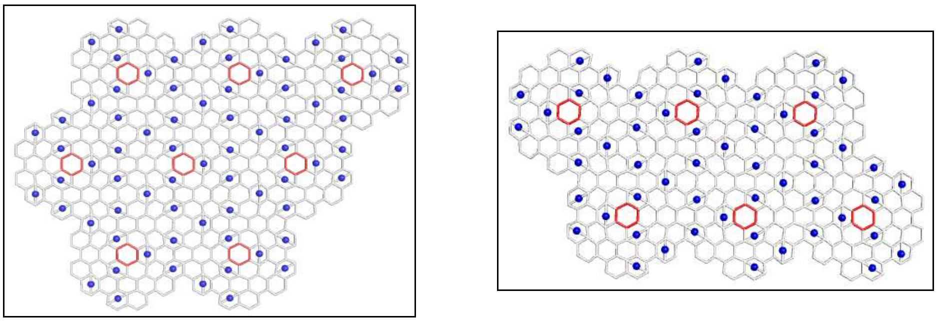

Figure 4. A cyclic domain $SuCor_8$, v=688 (left) and a parallelogram-like domain $P_{3,2}$, v=522 (right)

Examples are given in the table 1.

General formulas for W_n and B_n

In such a case, W_n is calculated by the formula:

$$\begin{aligned}
W_n &= W_{r_{k-1}} + \left\lfloor \frac{n-r_{k-1}}{k} \right\rfloor + 2\left(n - r_{k-1} - \left\lfloor \frac{n-r_{k-1}}{k} \right\rfloor \right) + (n - r_{k-1} - 1) = W_{r_{k-1}} + 3(n - r_{k-1}) - \left\lfloor \frac{n-r_{k-1}}{k} \right\rfloor - 1 \\
&= W_{r_{k-2}} + 3(r_{k-1} - r_{k-2}) - \left\lfloor \frac{r_{k-1}-r_{k-2}}{k-1} \right\rfloor + 3(n - r_{k-1}) - \left\lfloor \frac{n-r_{k-1}}{k} \right\rfloor - 1 \\
&= \cdots = W_{r_{k-k}} + 3(r_{k-(k+1)} - r_{k-k}) - \left\lfloor \frac{r_{k-(k+1)} - r_{k-k}}{k-(k+1)} \right\rfloor + \cdots + 3(n - r_{k-1}) - \left\lfloor \frac{n-r_{k-1}}{k} \right\rfloor - 1 \\
&= \left(\sum_{k=1}^{z} 3(r_k - r_{k-1}) - \left\lfloor \frac{r_k - r_{k-1}}{k} \right\rfloor \right) + \left(3(n - r_z) - \left\lfloor \frac{n - r_z}{z+1} \right\rfloor - 1 \right) \\
&= \left(\sum_{k=1}^{z} 18k - 6 \right) + \left(3(n - (3z(z+1)+1)) - \left\lfloor \frac{n - (3z(z+1)+1)}{z+1} \right\rfloor - 1 \right)
\end{aligned} \tag{9}$$

Similarly, for B_n we have:

$$\begin{aligned}
B_n &= B_{r_{k-1}} + \left(n - r_{k-1} - \left\lfloor \frac{n-r_{k-1}}{k} \right\rfloor \right) + (n - r_{k-1} - 1) \\
&= \left(\sum_{k=1}^{z} 12k - 6 \right) + \left(2(n - (3z(z+1)+1)) - \left\lfloor \frac{n - (3z(z+1)+1)}{z+1} \right\rfloor - 1 \right)
\end{aligned} \tag{10}$$

To find z in case $n > r_z$, (i.e., when the number of Sucor units are higher than in a complete cyclic domain D_z) we simply use the formula (3).

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An algorithm for compute Omega polynomial $\Omega(G,x)$ in the Sucor net can be written as: give *n*; find *z*; find W_n and B_n; if $n = 3z(z+1)+1$ then put $W_n = W_n + 1$ and $B_n = B_n + 1$; compute $\Omega(G,x)$

Omega polynomial in parallelogram domains $P_{a,b}$

In case of a parallelogram domain (Figure 4, right)) in Sucor net, the formulas are presented in the following.

$$W_{a,b} = (a-1)b + (2a-1)(b-1) = 3ab - 2a - 2b + 1 \quad (11)$$

$$B_{a,b} = 2(a-1)(b-1) = 2ab - 2a - 2b + 2 = W_{a,b} - ab + 1 \quad (12)$$

$$\begin{aligned}\Omega(G,x) &= (36n - 4W_{a,b} - 3B_{a,b})x + (9n - 3W_{a,b})x^2 + (12n + 2W_{a,b})x^3 + (3n - W_{a,b})x^4 \\ &+ (6n - 3B_{a,b})x^5 + (W_{a,b} + 3B_{a,b})x^6 \\ &= (36ab - 12ab + 8a + 8b - 4 - 6ab + 6a + 6b - 6)x + (9ab - 9ab + 6a + 6b - 3)x^2 \\ &+ (12ab + 6ab - 4a - 4b + 2)x^3 \\ &+ (3ab - 3ab + 2a + 2b - 1)x^4 + (6ab - 6ab + 6a + 6b - 6)x^5 \\ &+ (3ab - 2a - 2b + 1 + 6ab - 6a - 6b + 6)x^6 \\ &= (18ab + 14a + 14b - 10)x + (6a + 6b - 3)x^2 + (18ab - 4a - 4b + 2)x^3 \\ &+ (2a + 2b - 1)x^4 + (6a + 6b - 6)x^5 + (9ab - 8a - 8b + 7)x^6\end{aligned} \quad (13)$$

Examples are given in Table 1.

Table 1. Examples of Omega polynomial and CI in Sucor network

Domain	Omega polynomial	CI
D_7	$186X + 27X^2 + 108X^3 + 9X^4 + 24X^5 + 30X^6$	**806910**
D_{19}	$444X^1 + 45X^2 + 312X^3 + 15X^4 + 42X^5 + 114X^6$	**5866950**
D_{12}	$297X^1 + 36X^2 + 192X^3 + 12X^4 + 33X^5 + 63X^6$	**2353842**
D_{17}	$408X^1 + 45X^2 + 276X^3 + 15X^4 + 42X^5 + 96X^6$	**4709766**
P_{32}	$168X^1 + 27X^2 + 90X^3 + 9X^4 + 24X^5 + 21X^6$	**596490**
P_{44}	$391X^1 + 45X^2 + 258X^3 + 15X^4 + 42X^5 + 87X^6$	**4182894**

Numerical calculations were made by our software package Nano Studio [18].

CONCLUSIONS

Omega polynomial description proved to be a simple and efficient method in topological characterization of new designed nano-structures. Quantum calculations, to evaluate the stability of some small domains of the SuCor graphene are in progress in our. Lab and will be presented in a further article.

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