Scientific paper

Sumanene Units in P-type Surface Networks

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Abstract

Sumanene is a synthesized circulene molecule, with formula: $6:(5,6)_3$. We propose here units for periodic P-type surface networks, based on their stability, evaluated at the Hartree-Fock HF level of theory. Design of the yet hypothetical lattices was performed by using operations on maps, as provided by CVNET and Nano Studio software. The topology of the network was characterized by Omega polynomial.

Keywords: Sumanene, P-type surface networks, Omega polynomial.

1. Introduction

Among the carbon allotropes discovered in the nano-era, fullerenes (zero-dimensional), nanotubes (one dimensional), graphene (two dimensional) and spongy carbon (three dimensional) were the most challenging.[1,2] Inorganic compounds including oxides, sulfides, selenides, borates, silicates, etc. of many metals, also found applications as nano-structured functional materials.[3–12]

Zeolites are natural or synthetic alumino-silicates with an open three-dimensional crystal structure. Zeolites are micro-porous solids known as »molecular sieves.« The term molecular sieve refers to the property of these materials to selectively sort molecules, based primarily on a size exclusion process. This is due to a regular structure of pores, of molecular dimensions, forming channels.[13–17]

The rigorous and often aesthetically appealing architecture of crystal networks attracted the interest of scientists in a broad area, from crystallographers, to chemists and mathematicians.

The present study deals with some hypothetical carbon crystal-like nanostructures, based on real Sumanene molecule, of which stability is calculated at the Hartree-Fock HF level of theory and topology is described in terms of Omega polynomial.

2. Network Design

The hypothetical carbon crystal networks herein discussed were built up either by identifying two opposite open faces of a unit, as in Figure 1, left, or by joining the opposite atoms, as in Figure 1, middle and right, by the aid of Nano Studio software,[18] also enabling their embedding in the P-type surface,[1,2] which belongs to the space group P_n 3 m. The topological characterization will be done on cubic (k,k,k) domains (see Figure 2).

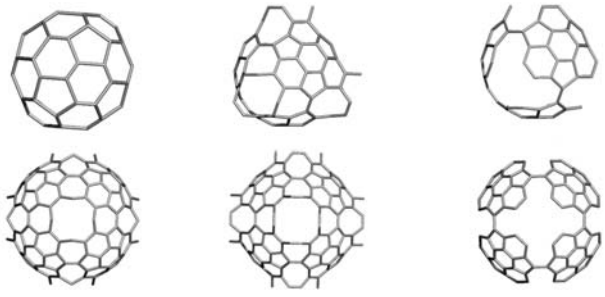

Figure 1. Top row: C60 (left), Sum_TA_108 (middle); Sum_T_84 (right). Bottom row: Sum_CZ_192 (left); Sum_CA_216 (middle); Sum_S2LeX_168 (right).

2. 1. Computational

The stability of periodic P-type surface networks were tested based on optimized geometries at Hartree-Fock HF (HF/6-31G**) level of theory. The calculations were performed in gas phase by Gaussian 09.[19] It was necessary to use relatively large computational effort for the examination, due to the size of the structures, used method and basis sets of calculations.

Within this work, stability tests of five units consisting of Sumanene patch (Figure 2) was carried out. As a reference structure, we considered C_{60}, the most referred structure in Nanoscience. Table 1 lists the total energy obtained after optimization of the analyzed structures at Hartree-Fock HF (HF/6-31G**) level of theory, the total energy per Carbon atom, E_{tot}/atom and HOMO-LUMO HL Gap. This test of stability was done to support the idea that sumanene, a real molecule, can be used to synthesize structural units for more elaborated nanostructures: Sum_T_A_108 (middle); Sum_T_84 for dendrimers while Sum_CZ_192, Sum_CA_216,and Sum_S_2LeX_168 for ordered Schwarzites, embedded in the P-surface. From Table 1 it is clear that such units show a stability comparable (or higher) to the well-known C_{60} reference structure; Sum_T_84 and Sum_S_2LeX_168 are the most simple and stable units, possible candidates for laboratory synthesis.

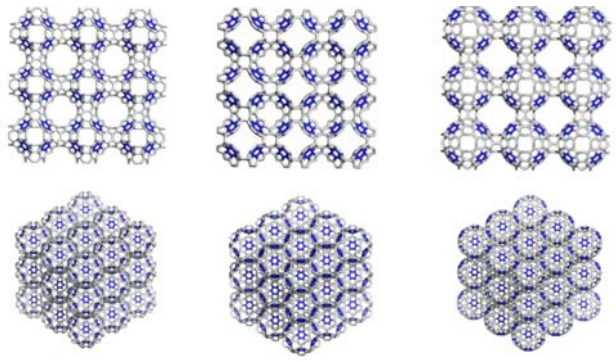

Figure 2. Top row: Sum_CA_216 (left), Sum_S2LeX_168 (middle); Sum_CZ_192 (right). Bottom row: the corresponding P-networks, in the corner position; k = 3.

Table 1. Total energy E_{tot} per atom (kcal/mol) and HOMO-LUMO HL Gap, at Hartree-Fock HF (HF/6-31G**) level of theory for some Sumanene-based units, possible to be used in construction of periodic structures.

	Structure	No. C atoms	HF/6-31G (d,p) (au)	E_{tot}/atom (au/mol)	HF_Gap (eV)
1	C_{60}	60	–2271.830	–37.864	7.418
2	Sum_TA_108	108	–4103.136	–37.992	7.259
3	Sum_T_84	84	–3194.384	–38.028	7.562
4	Sum_CZ_192	192	–7298.367	–38.012	6.044
5	Sum_CA_216	216	–8206.401	–37.993	6.442
6	Sum_S_2LeX_168	168	–6389.018	–38.030	6.637

We mention here that networks similar to those described above are frequently used as molecular sieves, and their structure was modeled.[20]

2. 2. Omega Polynomial

A counting polynomial[21] is a representation of a graph $G(V,E)$, with the exponent k showing the extent of partitions $p(G)$, $\cup\, p(G) = P(G)$ of a graph property $P(G)$ while the coefficient $p(k)$ are related to the number of partitions of extent k.

$$P(x) = \sum_k p(k) \cdot x^k \tag{1}$$

Let G be a connected graph, with the vertex set $V(G)$ and edge set $E(G)$. Two edges $e = (u,v)$ and $f = (x,y)$ of G are called *codistant* (briefly: *e co f*) if the notation can be selected such that:[22]

$$d(v,x) = d(v,y) + 1 = d(u,x) + 1 = d(u,y) \tag{2}$$

where d is the usual shortest-path distance function. The above relation *co* is reflexive (*e co e*) and symmetric (*e co f*) for any edge e of G but in general is not transitive.

A graph is called a *co-graph* if the relation *co* is also transitive and thus an equivalence relation.

Let $C(e)$: = $\{f \in E(G); f\ co\ e\}$ be the set of edges in G that are codistant to $e \in E(G)$. The set $C(e)$ can be obtained by an orthogonal edge-cutting procedure.: take a straight line segment, orthogonal to the edge e, and intersect it and all other edges (of a polygonal plane graph) parallel to e. The set of these intersections is called an *orthogonal cut* (*oc* for short) of G, with respect to e.

If G is a *co-graph* then its orthogonal cuts C_1, C_2, ..., C_k form a partition of $E(G) = C_1 \cup C_2 \cup ... \cup C_k$, $C_i \cap C_j = \varnothing$, $i \neq j$.

A subgraph $H \subseteq G$ is called *isometric*, if $d_H(u, v) = d_G(u, v)$, for any $(u, v) \in H$; it is *convex* if any shortest path in G between vertices of H belongs to H. The relation *co* is related to ~ (Djoković[23]) and Θ (Winkler[24]) relations.[25,26]

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. Note that John *et al.*[22] implicitly used the "*op*" relation in defining the Cluj-Ilmenau index *CI*.

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 choice about the maximum size of

face/ring, and the face/ring mode counting, will decide the length of the strip.

Also note that *ops* are *qoc* (quasi orthogonal cuts), meaning the transitivity relation is, in general, not obeyed.

The Omega polynomial[27–29] $\Omega(x)$ is defined on the ground of opposite edge strips *ops* 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

$$\Omega(x) = \sum_s m \cdot x^s \tag{3}$$

The first derivative (in $x = 1$) can be taken as a graph invariant or a topological index:

$$\Omega'(1) = \sum_s m \cdot s = |E(G)| \tag{4}$$

An index, called Cluj-Ilmenau[22] $CI(G)$, was defined on $\Omega(x)$:

$$CI(G) = \{[\Omega'(1)]^2 - [\Omega'(1) + \Omega''(1)]\} \tag{5}$$

In tree graphs, the Omega polynomial simply counts the non-opposite edges, being included in the term of exponent $s = 1$. A similar description of polyhedral nanostructures can be done by using the Cluj polynomial.[30]

2. 3. Omega Polynomial in Sumanene-based Networks

Omega polynomials are herein calculated at various R_{max}. Formulas were derived by numerical analysis. Formulas for the infinite networks are listed in Tables 2 to 7, with examples at the bottom of these tables.

Formulas for the number of vertices and number of various rings are given in Tables 8 and 9, respectively.

Table 2. Omega polynomials in **Sum_CA_216,"N"**; **R_{max}[6]**

Formulas			
$\Omega(G, x) = [k^2(72k + 60)]x^1 + [k^2(72k - 24)]x^2 + 24k^2 x^3 + [12k^2 (k - 1)]x^6$			
$\Omega'(G, 1) = \|E(G)\| = 288k^3 + 12k^2 = 12k^2 (24k + 1)$			
$CI(G) = 82944k^6 + 6912k^5 + 144k^4 - 792k^3 + 252k^2$			
k	**Omega polynomial: examples**	***e*(*G*)**	**C*I*(*G*)**
1	$132x^1 + 48x^2 + 24x^3$	300	89460
2	$816x^1 + 480x^2 + 96x^3 + 48x^6$	2352	5526576
3	$2484x^1 + 1728x^2 + 216x^3 + 216x^6$	7884	62138340
4	$5568x^1 + 4224x^2 + 384x^3 + 576x^6$	18624	346806720
5	$10500x^1 + 8400x^2 + 600x^3 + 1200x^6$	36300	1317597300
6	$17712x^1 + 14688x^2 + 864x^3 + 2160x^6$	62640	3923607600

Table 3. Omega polynomials in **Sum_CA_216, "N"; R_{max}[8]**

Formulas			
$\Omega(G, x) = 48k^2 x^2 + [12k(2k + 1)]x^3 + [24k^2(2k - 1)]x^4 + [12k(k - 1)]x^5 + [12k^2(k - 1)]x^6 + [3k(k - 1)^2]x^8$			
$\Omega'(G, 1) = \|E(G)\| = 288k^3 + 12k^2 = 12k^2 (24k + 1)$			
$CI(G) = 82944k^6 + 6912k^5 + 144k^4 - 1392k^3 + 492k^2$			
k	**Omega polynomial: examples**	***e*(*G*)**	**C*I*(*G*)**
1	$48x^2 + 36x^3 + 24x^4$	300	89100
2	$192x^2 + 120x^3 + 288x^4 + 24x^5 + 48x^6 + 6x^8$	2352	5522736
3	$432x^2 + 252x^3 + 1080x^4 + 72x^5 + 216x^6 + 36x^8$	7884	62124300
4	$768x^2 + 432x^3 + 2688x^4 + 144x^5 + 576x^6 + 108x^8$	18624	346772160
5	$1200x^2 + 660x^3 + 5400x^4 + 240x^5 + 1200x^6 + 240x^8$	36300	1317528300
6	$1728x^2 + 936x^3 + 950x^4 + 360x^5 + 2160x^6 + 450x^8$	62640	3923486640

Table 4. Omega polynomials in **Sum_S$_2$LeX_168, "X"**; **R$_{max}$[6]= R$_{max}$[8]**

Formulas			
$\Omega(G, x) = 60k^3 x + 48k^3 x^2 + 24k^2 x^3 + 12k^2 (k-1) x^5$			
$\Omega'(G, 1) = \|E(G)\| = 216k^3 + 12k^2 = 12k^2 (18k + 1)$			
$CI(G) = 46656k^6 + 5184k^5 + 144k^4 - 552k^3 + 84k^2$			
k	**Omega polynomial: examples**	***e*(*G*)**	**C*I*(*G*)**
1	$60x^1 + 48x^2 + 24x^3$	228	51516
2	$480x^1 + 384x^2 + 96x^3 + 48x^5$	1776	3150096
3	$1620x^1 + 1296x^2 + 216x^3 + 216x^5$	5940	35269452
4	$3840x^1 + 3072x^2 + 384x^3 + 576x^5$	14016	196414272
5	$7500x^1 + 6000x^2 + 600x^3 + 1200x^5$	27300	745223100
6	$12960x^1 + 10368x^2 + 864x^3 + 2160x^5$	47088	2217163536

Table 5. Omega polynomials in **Sum_S$_2$LeX_168, "X"**; **R$_{max}$[10]**

Formulas			
$\Omega(G, x) = [k(48k^2 + 88k - 17)]x^1 + [30k^3 - 9k^2 + 4k + 2]x^2 + [2k(10k^2 - 11k + 7)]x^3 + [k(3k^2 + k - 3)]x^4 + [k(3k^2 - k - 2)]x^5 + [k(k-1)^2]x^6 + [k(k^2 - 2k + 2)]x^7 + [k^3 + k^2 - 17k + 2]x^8 + [3k(k-1)]x^9 + [2(k-1)]x^{10}$			
$\Omega'(G, 1) = \|E(G)\| = 216k^2 + 12k^2 = 12k^2 (18k + 1)$			
$CI(G) = 46656k^6 + 5184k^5 + 144k^4 - 620k^3 + 18k^2 + 74k + 64$			
k	**Omega polynomial: examples**	***e*(*G*)**	**C*I*(*G*)**
1	$119x^1 + 27x^2 + 12x^3 + 1x^4 + 1x^7 + 1x^8$	228	51520
2	$702x^1 + 214x^2 + 100x^3 + 22x^4 + 16x^5 + 2x^6 + 4x^7 + 8x^8 + 6x^9 + 2x^{10}$	1776	3149500
3	$2037x^1 + 743x^2 + 384x^3 + 81x^4 + 66x^5 + 12x^6 + 15x^7 + 29x^8 + 18x^9 + 4x^{10}$	5940	35267308
4	$4412x^1 + 1794x^2 + 984x^3 + 196x^4 + 168x^5 + 36x^6 + 40x^7 + 70x^8 + 36x^9 + 6x^{10}$	14016	196409224
5	$8115x^1 + 3547x^2 + 2020x^3 + 385x^4 + 340x^5 + 80x^6 + 85x^7 + 137x^8 + 60x^9 + 8x^{10}$	27300	745213384
6	$3434x^1 + 6182x^2 + 3612x^3 + 666x^4 + 600x^5 + 150x^6 + 156x^7 + 236x^8 + 90x^9 + 10x^{10}$	47088	2217146980

Table 6. Omega polynomials in **Sum_CZ_192, "Z"**; **R$_{max}$[6]**

Formulas			
$\Omega(G, x) = [12k^2(10k-1)]x + 48k^3 x^2 + 24k^3 x^3$			
$\Omega'(G, 1) = \|E(G)\| = 288k^3 + 12k^2 = 12k^2 (24k - 1)$			
$CI(G) = 46656k^6 + 5184k^5 + 144k^4 - 552k^3 + 84k^2$			
k	**Omega polynomial: examples**	***e*(*G*)**	**C*I*(*G*)**
1	$108x^1 + 48x^2 + 24x^3$	276	75660
2	$312x^1 + 384x^2 + 192x^3$	2256	5085360
3	$3132x^1 + 1296x^2 + 648x^3$	7668	58784076
4	$7488x^1 + 3072x^2 + 1536x^3$	18240	332664000
5	$14700x^1 + 6000x^2 + 3000x^3$	35700	1274424300
6	$25488x^1 + 10368x^2 + 5184x^3$	61776	3816160560

Table 7. Omega polynomials in **Sum_CZ_192, "Z"**; **R$_{max}$[8]**

Formulas			
$\Omega(G, x) = [12k^2 (5k+4)]x + [24k^2 (3k-1)]x^2 + 24k^2 x^3 + [3k^2 (k-1)]x^4 + [3k^2 (k-1)]x^4 + [12k^2 (k-1)]x^6$			
$\Omega'(G, 1) = \|E(G)\| = 288k^3 + 12k^2 = 12k^2 (24k + 1)$			
$CI(G) = 82944k^6 - 6912k^5 + 144k^4 - 828k^3 + 312k^2$			
k	**Omega polynomial: examples**	***e*(*G*)**	**C*I*(*G*)**
1	$18x^1 + 48x^2 + 24x^3$	276	75660
2	$672x^1 + 480x^2 + 96x^3 + 12x^4 + 48x^6$	2256	5084160
3	$2052x^1 + 1728x^2 + 216x^3 + 54x^4 + 216x^6$	7668	58778676
4	$4608x^1 + 4224x^2 + 384x^3 + 144x^4 + 576x^6$	18240	332649600
5	$8700x^1 + 8400x^2 + 600x^3 + 300x^4 + 1200x^6$	35700	1274394300
6	$14688x^1 + 14688x^2 + 864x^3 + 540x^4 + 2160x^6$	61776	3816106560

Table 8. Number of atoms $v = |V(G)|$

$v(N) = 8k^2[27 + 24(k-1)]$	$v(X) = 8k^2[21 + 18(k-1)]$	$v(Z) = 192k^3$
k	**N**	**X**	**Z**
1	216	168	192
2	1632	1248	1536
3	5400	4104	5184
4	12672	9600	12288
5	24600	18600	24000
6	42336	31968	41472

Table 9. Number of rings

$R[5](N) = 24k^3$; $R[6](N) = 4k^2[8 + 11(k-1)]$; $R[8](N) = 26k^3$
$R[5](X) = 24k^3$; $R[6](X) = 32k^3$; $R[8](N) = 2k^3$
$R[5](Z) = 24k^3$; $R[6](Z) = 32k^2$; $R[8](Z) = 2k^2[8 + 7(k-2)]$

k	**N**			**X**			**Z**		
	R[5]	**R[6]**	**R[8]**	**R[5]**	**R[6]**	**R[8]**	**R[5]**	**R[6]**	**R[8]**
1	24	32	26	24	32	–	24	32	–
2	192	304	208	192	256	16	192	256	64
3	648	1080	702	648	864	54	648	864	270
4	1536	2624	1664	1536	2048	128	1536	2048	704
5	3000	5200	3250	3000	4000	250	3000	4000	1450
6	5184	9072	5616	5184	6912	432	5184	6912	2592

4. Conclusions

In this paper, we presented the design of three hypothetical carbon networks, embedded in the P-type surface, achieved by the aid of Nano Studio software. The stability of these units, as given by the Hartree-Fock calculations, was found to be close to that of the C_{60} reference structure, thus being a promise for the laboratory synthesis. The topology of these networks was characterized by Omega counting polynomial, at various maximal rings. The number of vertices and rings in such infinite carbon nanostructures was also given.

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Povzetek

Sumanen je sintetična cirkulenska molekula s formulo $6{:}(5,6)_3$. V tem delu predlagamo enote za periodične P-tipe površinskih mrež glede na njihovo stabilnost, ki jo izračunamo z uporabo Hartree-Fock HF teorije. Zaenkrat še hipotetične površinske mreže smo načrtovali s pomočjo teorije operatorjev na preslikavah, ki je vgrajena v CVNET and Nano Studio računalniška programa. Topologijo površinskih mrež smo popisali z Omega polinomi.