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Topology of C_{20} Based Spongy Nanostructures

Mircea V. Diudea[1], **Beata Szefler**[2*]

[1]*Department of Chemistry, Faculty of Chemistry and Chemical Engineering*
Babes-Bolyai University, 400028 Cluj, Romania

[2]*Department of Physical Chemistry, Collegium Medicum*
Nicolaus Copernicus University, Kurpińskiego 5, 85-096, Bydgoszcz, Poland
[*]*E-mail: beatas@cm.umk.pl*

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Abstract: Spongy materials are encountered in nature in zeolites used as molecular sieves. There are also synthetic compounds like spongy carbon, metal-organic frameworks MOFs, etc, with a hollow structure. The design and topological study of some hypothetical spongy nanostructures is presented in terms of map operations and genus calculation on their associated graphs. The design of nanostructures was performed by original software packages.

Key words: polyhedral cage, spongy structure, genus

I. INTRODUCTION

Spongy structures are hollow-containing materials encountered in natural or synthesized zeolites, in spongy carbon, etc., spongy polyhedra that can evolve with 1-periodicity or radially to provide multi-shell cages. Spongy multi-shell cages are also called multi-tori, because they consist of more than one torus [1-4]. They include negatively curved substructures [5-8] and are also termed *schwarzites*, in honor of H.A. Schwarz [9,10] who firstly investigated the differential geometry of such kind of surfaces. Multi-tori are supposed to result by self-assembling of some repeating units/monomers formed by opening of cages/fullerenes.

Graphs associated to schwarzites are assumed to be embedded in triply periodic (intersection-free) minimal surfaces thus forming labyrinth graphs. A surface S can be characterized by its genus [11,12], defined in terms of the integral Gaussian curvature according to the Gauss-Bonnet relation [13]

$$\chi(S) = (1/2\pi) \int_S K \mathrm{d}S \qquad (1)$$

with $\chi(S)$ being the Euler-Poincaré characteristic. From this, the surface genus g is calculated by the Euler-Poincaré formula [12]:

$$\chi(S) = n(1-g) = v - e + f \qquad (2)$$

where $n = 1$ for non-orientable (Moebius) surfaces and $n = 2$ for orientable surfaces while $v = |V(G)|$ is the number of vertices/atoms, $e = |E(G)|$ is the number of edges/bonds and f is the number of faces of the graph/molecule.

II. OPERATIONS ON MAPS

A map *M* is a combinatorial representation of a (closed) surface. Operations on maps are topological-geometrical transformations allowing to transform or to relate a given polygonal structure. Several operations on maps are known and we present herein only the most used ones [14-18].

Dualization Du of a map starts by locating a point in the center of each face (Fig. 1, left). Next, two such points are joined if their corresponding faces share a common edge

(Fig. 1, right). It is the (Poincaré) *dual Du*(*M*). The vertices of *Du*(*M*) represent the faces of *M* and *vice-versa.* Thus the following relations exist: *Du*(*M*); $v = f_0$; $e = e_0$; $f = v_0$ [19].

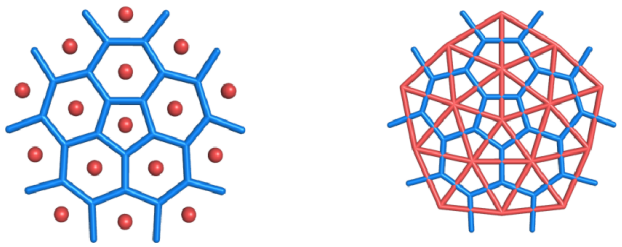

Fig. 1. Dualization of a fullerene patch

Dual of the dual returns the original map: $Du(Du(M)) = M$. Tetrahedron is self-dual while the other Platonic polyhedra form pairs: Du (Cube (C)) = octahedron (Oct); Du (Dodecahedron (Do)) = Icosahedron (Ico) (Fig. 2). Note that all the operation parameters presented herein refer to regular maps (e.g., the Platonic solids); a subscript zero indicates a parent map parameter.

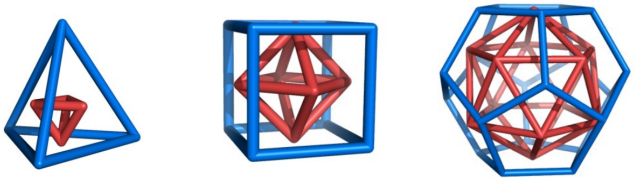

Fig. 2. The duals of the five Platonic polyhedra

Polygonal P_k ***mapping*** ($k = 3,\ 4,\ 5$) of a face is achieved as follows [2, 3]: add a new vertex in the center of the face. Put $k - 3$ points on the boundary edges (Fig. 3). Connect the central point with one vertex (the end points included) on each edge. In this way the parent face is covered by triangles ($k = 3$), quadrilaterals ($k = 4$) and pentagons ($k = 5$). The P_3 operation is also called *stellation* or (centered) *triangulation*. The resulting map shows the relations: $P_k(M)$, $v = v_0 + (s - 3)e_0 + f_0$; $e = se_0$; $f = s_0 f_0$, so that the Euler's relation (2) holds. Fig. 4 gives examples of the P_k operations realization.

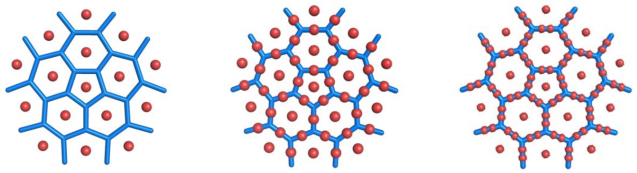

Fig. 3. Polygonal mapping of a fullerene patch; P_3 (left); P_4 (middle) and P_5 (right)

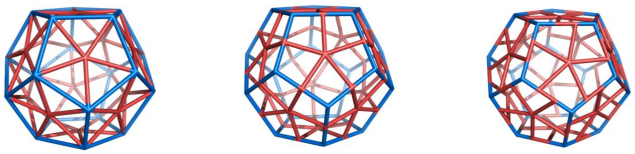

Fig. 4. Polygonal mapping of the Dodecahedron by P_3(Do) (left); P_4(middle) and P_5(Do) (right)

Medial Med of a map is achieved [2,19] by putting a new vertex in the middle of each original edge. Join two vertices if the original edges span an angle (and are consecutive within a rotation path around their common vertex in M) Fig 5. Medial is a 4-valent graph and $Med(M) = Med(Du(M))$. The transformed parameters are: $Med(M)$; $v = e_0$; $e = 2e_0$; $f = f_0 + v_0$.

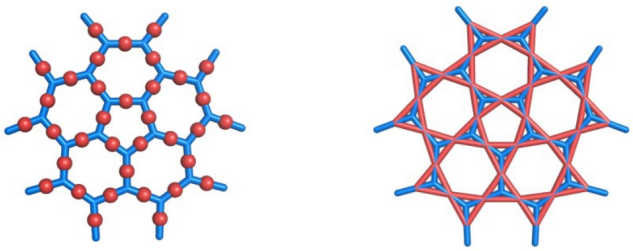

Fig. 5. Medial of a fullerene patch

Medial operation rotates parent s-gonal faces by π/s. Points in the medial represent original edges, thus this property can be used in topological analysis of edges in the parent polyhedron. Similarly, the points in dual give information on the topology of parent faces. Fig. 6 illustrates the *medial* operation performed on the five Platonic polyhedra.

Fig. 6. The medials of the five Platonic polyhedra

Truncation Tr is achieved [2, 19] by cutting off the neighborhood of each vertex by a plane close to the vertex, such that it intersects each edge incident to that vertex. Truncation is similar to the medial, the transformed parameters being: $Tr(M)$; $v = 2e_0 = d_0 v_0$; $e = 3e_0$; $f = f_0 + v_0$. This was the main operation used by Archimedes in building up the well-known 13 (Archimedean) solids. Fig. 7 illustrates the realization of this operation on the Icosahedron.

Tab. 1. Genus calculation in spongy structures $C_n(Do_n)$ of Fig. 1

Structure	v	e	f_5	$f_w(s)^*$	f	χ	g	g_u	u
$C_4(Do_4)$_50	50	90	42	4(3)	36	-4	3	1.5	4
$C_8(Do_8)$_100	100	180	84	6(4)	72	-8	5	1.5	8
$C_{20}(Do_{20})$_250	250	450	222	12(5)	180	-20	11	1.5	20

$^*f_w$ stands for the window-faces

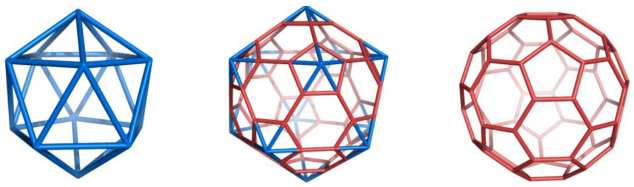

Fig. 7. Truncation of the Icosahedron

III. STRUCTURE CONSTRUCTION

Dodecahedron Do, as the molecule C_{20}, can self-arrange in spongy structures of general formula $C_n(Do_n)$, with C_n being a tri-connected cage submitted to map operations (a map is a discretized surface) as follows: (*i*) design the *hollow core* by applying the polygonal P_4 map operation on C_n (that covers the map with square-like faces) followed by the selective truncation "TRS" of the highest-connected vertices; (*ii*) draw the *envelope* by $S_2(C_n)$ map operation [18]. Next, the two cages: $P_4TRS(C_n)$ (inside) and $S_2(C_n)$ (outside) are interconnected (by joining the closest pair atoms) to give $C_n(P_4TRS@S_2)(Do_n)$ or simply $C_n(Do_n)$. The number of atoms in such spongy double-shell cages [4] is $n_{\text{spongy}} = 12.5n$ and it is often written as a suffix: $C_n(Do_n)$_$12.5n$. For the three cubic Platonic solids, the corresponding objects are shown in Fig. 8.

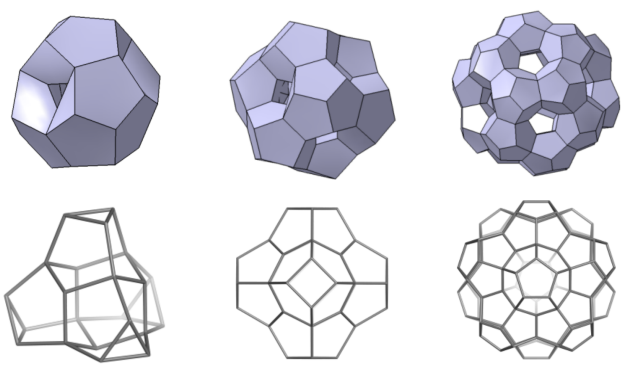

Fig. 8. Spongy structures decorated by dodecahedron Do cages, derived from the Platonic solids: dodecahedron (Do=C_{20}, top); cube (C=C_8, middle) and tetrahedron (T=C_4, bottom)

In spongy structures, *built up from u tube junction units, of genus g_u, the genus is calculated by:*

$$g = u(g_u - 1) + 1 \qquad (3)$$

irrespective of the unit tessellation [20]. For the spongy structures of Fig. 8, the genus is calculated cf. (3), as shown in Tab. 1.

The spongy structure $C_{20}(Do_{20})$_250 (Fig. 8, right) is a 6-nodal 3,4-c $\left\{(5^6)_{60}\left[(5^5)_{30}(5^5)_{60}\right]\left[(5^3)_{20}(5^3)_{20}(5^3)_{60}\right]\right\}$ spongy hyper-dodecahedron, made from 20 cells all dodecahedral, a face-regular $5R_5$ map of genus $g = 11$, its core being the 110-keplerate [4]. The packing fraction $\phi = 20/33 \approx 0.6060$ is calculated with respect to the 33 dodecahedra needed for the radial space filling). Comparing with the spheres maximum fraction (0.7405) clearly it is a spongy, non-convex structure. Its pentagons, however, show some distortion (and strain) to the regular pentagon. For the general regular polytopes the reader is invited to consult refs. [21-24].

IV. CONCLUSIONS

Spongy structures were designed in this paper by using map operations, as implemented in our original software packages CVNET and Nano Studio. The genus calculation of their associated graphs revealed that these are structures of high genera. Structures have been done by our original software CVNET and Nano Studio [25,26].

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Mircea V. Diudea – professor of chemistry at the Department of Chemistry, Faculty of Chemistry and Chemical Engineering, "Babes-Bolyai" University, Arany Janos Str. 11, 400028, Cluj, Romania. Research interests: molecular modeling of fullerenes, graphenes, crystal and quasicrystal networks design, aromatic systems, QSAR, Mathematical Chemistry and Molecular Topology (matrices, topological indices, polynomials). Publications: more than 300 articles, book chapters, 15 books (authored or edited), 65 conference presentations, index $H > 28$.

Beata Szefler – doctor of chemistry, laboratory diagnostician, assistant professor at CM UMK in Bydgoszcz, Department of Physical Chemistry, Poland. Graduate of the Medical Academy in Bydgoszcz, Faculty of Pharmacy. Degree: PhD (2010) in Chemical Sciences, University of Technology & Life Sciences Bydgoszcz, Poland. Experience in Microbiology, Hematology and Pharmacokinetics. Research interests: molecular modeling of aromatic systems, with particular emphasis on the importance of biochemical molecules, study on properties of fullerenes using HF, DFT methods and MD, docking ligand-protein, QSAR, crystallographic drug network. Principal investigator – parameterization of force fields, molecular dynamics simulations of selected protein and ligand-protein systems, quantum-chemical study of small ligands, topological properties of molecules, topological indices as descriptors in QSAR, drugs crystallography.