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Intermolecular interactions in pyridinium – anion – β -hexachlorocyclohexane molecular crystals

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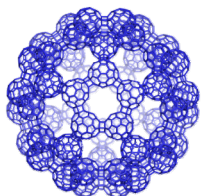
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In our recent work [1], we have shown that the simple ring structure of β -hexachlorocyclohexane (β -HCH) can act as halide anion acceptor. Accordingly, in this work, we have investigated the nature of intermolecular interactions in different molecular crystal configurations formed by pyridinium cation, chloride or bromide anion as well as β -hexachlorocyclohexane (β -HCH) molecules using high level *ab initio* quantum chemistry methods. Several molecular subsystems taken from the crystal unit cell were considered and their supramolecular energy stability was analyzed in detail using high level density-fitting local electron correlation (DF-LMP2 and DF-LCCSD(T)) methods together with the aug-cc-pVTZ basis set. In order to elucidate the nature of the intermolecular interactions between different fragments, the symmetry adapted perturbation theory (SAPT) method up to “2+3” truncation expansion was applied. The SAPT analysis has shown that the “simple” pair model of halide anion – β -HCH complex is not adequate to properly describe the stability of the crystals, since the charge polarization induced by the cation counterpart on the halide anion significantly changes the nature and the magnitude of the anion – β -HCH interaction.

Keywords: molecular crystals, intermolecular interactions, halide anions, SAPT theory

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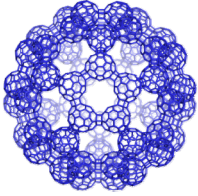
ORDERING CHEMICAL TREES BY WIENER POLARITY INDEX

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Suppose G is a chemical graph G with vertex set $V(G)$. The Wiener polarity index $W_p(G)$ is the number of unordered pairs of vertices $\{u, v\}$ such that $d_G(u, v) = 3$. Here, $d_G(u, v)$ denotes the length of a minimal path connecting u and v . In this talk, we report our recent results in computing the Wiener polarity index of chemical graph.

Keywords: Chemical graph, Wiener polarity index, graph operation.



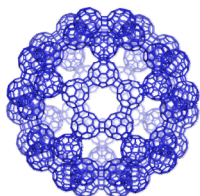
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A graph theoretical for analyzing DNA sequences based on codons

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Since Watson and Crick proposed the helical structure of DNA, many problems about this structure are posed. An important problem is how to read and recognize primary structure of a DNA sequence. One particular way to analyze DNA sequences and their properties is by using the concept of graph theory. Nanopore sequencing is a method under development for determining the order in which nucleotides occur on a strand of DNA. Nanopore devices are used in DNA sequencing with the hopes of enabling large and complete strands of DNA to be read completely. In this talk, we will present a new graph theoretical approach for reading a DNA sequence with nanopores. And also we will discuss about graphical and numerical representations of DNA sequences based on codons. As we know, in the recent years, a rapid growth of sequence data in DNA databases has been observed and it is difficult to obtain information directly from the primary sequences. Then mathematical analysis of the large volume of sequences data becomes one of the challenges for bio-scientists. Using graphical approaches to study biological problems can provide intuitive picture or useful insights for helping analyzing complicated relations in these systems.



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Abstract of lecture by Subhash C. Basak: International Academy of Mathematical Chemistry (IAMC) conference, Cluj, Romania, 2017, June 28-30.

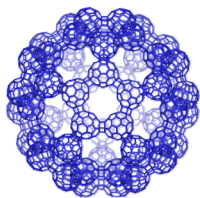
Title: Mathematical descriptors of molecules and biomolecules: Development and applications to characterization of chemical libraries, QSAR, drug design, nanotoxicology, and Zika peptide vaccine design

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During the past half century or so, we have witnessed numerous applications of discrete mathematics in the characterization of chemical and biological systems. Two principal factors sustained such a growth: i) Novel applications of discrete mathematics to chemical and biological systems, and ii) Availability of high speed computers and associated software whereby hypothesis driven as well as discovery oriented research could be carried out within a reasonable time frame. An individual descriptor maps the structure of the object under consideration to the real line \mathbb{R} . Whereas in the 1970s only a few descriptors could be calculated, currently available software can compute many descriptors for molecules or biomolecules like DNA/ RNA, proteins. Many of the chemodescriptors (those calculated for small molecules) and biodescriptors (computed for biomolecules like DNA/ RNA) are strongly correlated with one another. When p molecular descriptors are calculated for n objects, the data set can be viewed as n vectors in p dimensions, each molecule/ biomolecule being represented as a point in \mathbb{R}^p . Because descriptors are often strongly correlated with one another, the n points in \mathbb{R}^p will lie on a subspace of dimension lower than p . This lecture will cover the following aspects of developments and applications of chemodescriptors and biodescriptors:

- a) Characterization of intrinsic dimensionality of structure spaces arising out of calculated molecular descriptors and use of such descriptors in quantitative structure-activity relationship (QSAR) of large and diverse

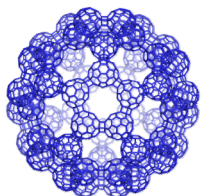


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- data sets related to drug discovery and hazard assessment of pollutants (1-6),
- b) Use of mathematical chemodescriptors in the design of drugs against malaria via a combination of pharmacophore modeling and mathematical descriptors on a proprietary library of >300,000 structures (7).
 - c) Mathematical characterization of nanotoxicoproteomics maps derived from multi-walled carbon nanotubes (MWCNT) and TiO₂ nanobelts (TiO₂-NB) treated cells (8).
 - d) Applications of mathematical sequence descriptors in the design of peptide vaccines active against global pathogens like Zika virus (ZIKV) and characterization of emerging viruses (9, 10).

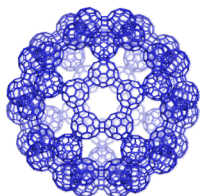
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Additive, multiplicative, and additive-multiplicative structure-property models. Which perform better?

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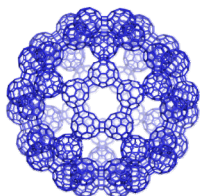
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Structure-property relationships (SARs) are mathematical models linking a property of a chemical compounds with structural descriptors. Frequently the SARs are linear regression models, which have several assumptions that need verification prior to model construction (such as normal distribution of the outcome variable – property in this case). A new family of descriptors has been recently introduced based on extending characteristic polynomial formula (ChPE). A theoretical study to investigate the link between ChPE descriptors and several properties of C₂₀ fullerene congeners (45 distinct structures) was conducted. Additive ($\hat{Y}=a+b_1*D+b_2*D'$, a =intercept, b_i =coefficients, D , D' =ChPE descriptors), multiplicative ($\hat{Y}=a+b*D*D'$), and additive-multiplicative ($\hat{Y}=a+b_1*D+b_2*D'+b_3*D*D'$) models with two ChPE descriptors were identified with a dedicated program. To identify the best performing model an adjusted determination coefficient was calculated by applying the formula: $r^2_{adj}=r^2-(1-r^2)\cdot k_D/(m-k_C)$, where r^2 =determination coefficient, m =number of compounds in the dataset (equal with 45 for C₂₀ fullerene), k_D =number of structural ChP descriptors (equal with 2), k_C =number of the coefficients included in the model. The comparison in regards of the explanatory power between additive, multiplicative, and additive-multiplicative models for a given equation relating a certain property was done with the studentized version of the Fisher Z transformation where $t(r^2_{adj})=atanh(\sqrt{r^2_{adj}})$, $\sigma(r^2_{adj})=(\sqrt{(m-3)})^{-1}$, $t_{i,j}=(t_i-t_j)/(\sqrt{\sigma^2_i+\sigma^2_j})$. Graphical representations are used for visual check of the models performances.

Keywords: structure-property relationship (SAR), models comparison, Extended Characteristic Polynomial Family of Descriptors (ChPE), theoretical study, C₂₀ fullerene congeners

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Revisiting the Methods of the Atomic Structure. Back to the Basis.

Fanica Cimpoesu

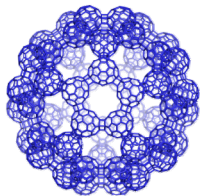
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It is well acknowledged that the Gaussian Type Orbitals (GTOs) are not natural primitives to build approximations of the atom electronic structure, first of all, because of the $\exp(-\alpha r^2)$ pattern, while Slater Type Orbitals (STOs), with $\exp(-\alpha r)$ exponential components are more appropriate to this goal. However, the GTOs are accepted as compromise for easier calculations of the atomic and molecular integrals, since the dawn of quantum chemistry.

At the same time, a hidden drawback, overlooked by the quasi-unanimity of users and developers of quantum chemistry programs, stays in the fact that the standardized GTO bases have drastic limitations in the radial polynomial co-factors. Thus, all the s-type GTOs are exclusively collections of $\exp(-\alpha r^2)$ functions, all the p-type ones consist in $r \cdot \exp(-\alpha r^2)$ components, while the d-type sets based on $r^2 \cdot \exp(-\alpha r^2)$ sets, and so on. Then, for instance, the lack of any r -type factor for the s-orbitals makes very problematic the retrieval of correct long range dependence of medium and high quantum numbers. The situation is similar for all types of GTO-based atomic orbitals.

A easy alleviation of the situation can be achieved introducing general $r^{n-1} \cdot \exp(-\alpha r^2)$ primitives for all the types of atomic shells, in analogy to the well-known $r^{n-1} \cdot \exp(-\alpha r)$ pattern of STO bases. Thus, in spite of the tacit belief that all the methodologic backgrounds are nowadays clarified, it seems that there is yet room to rework some essential issues on in the mathematical blueprints of the applied quantum chemistry.

Keywords: *atomic wave functions, basis sets, Gaussian-type orbitals*



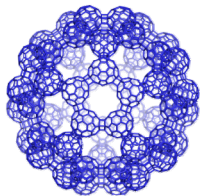
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PROPELLANES – A NEW CLASS OF STRUCTURES

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Design and properties of a new class of rhomb-tessellated structures, called Propellanes, ppl, is described. A structure is propellane if all the following conditions are fulfilled: (a) All strong rings are squares/rhombs; (b) Vertex classes consist of all non-connected vertices; (c) Line graph (i.e., Medial) of the original graph shows a Hamiltonian circuit; (d) Omega polynomial has a single term: $1X^{|E|}$.



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Computing degeneracies of the most important standard structures of polycyclic aromatic hydrocarbons

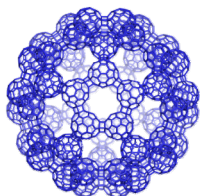
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For a given polycyclic aromatic hydrocarbon its **standard structure** is defined as a structure that

- does not have aromatic sextets, and
- has the smallest possible number of unpaired electrons.

Each aromatic sextet decreases by 90 kJ/mol the energy of the standard structure, while each pair of unpaired electrons increases the energy by 272 kJ/mol. The structures with the smallest energy are called the **most important structures**. The number of structures with the same energy is called the **degeneracy** of that structure.

We investigate the degeneracies of the top-most important structures for several classes of polycyclic aromatic compounds. In particular, we establish bijections with some well-known combinatorial structures and obtain closed-form expressions for some special cases.



STUDING SOME THERMODYNAMIC PROPERTIES OF OLIGOACENES USING FORGOTTEN INDEX

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Homologous classes of Polycyclic Aromatic Hydrocarbons (PAHs) play significant role as promising benefit for organic electronics and optoelectronic. One of these classes is Oligoacenes.

A topological index (also known as molecular descriptor) is any function on a graph that does not depend on a labeling of its vertices. One of these degree based graph invariants is forgotten index which is introduced by Furtula and Gutman. In this paper, we will increase the physico-chemical applicability of the forgotten index. Firstly, we present explicit formula of Forgotten index of Oligoacenes family and then a model to predict some thermodynamic properties through forgotten index. All information about the first members of Oligoacenes family were derived from reliable experimental data and valid references.

Keywords: Polycyclic Aromatic Hydrocarbons, Oligoacene, Forgotten index.

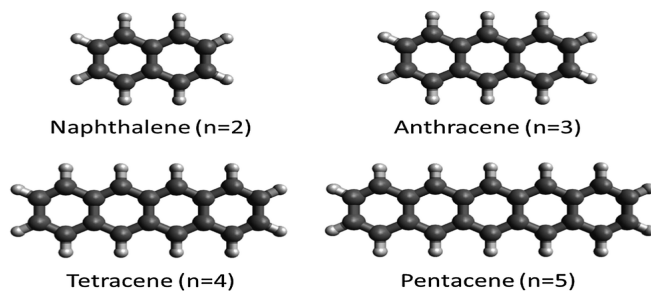
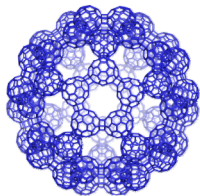


Figure. Oligoacenes family ($n = 2$ to 5)

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Symmetry of Cubic Graphs

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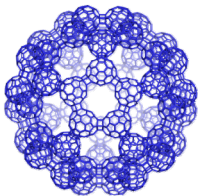
A weighted graph $G = (V, E, w, \lambda)$ is a combinatorial object consisting of an arbitrary set $V = V(G)$ of vertices, a set $E = E(G)$ of unordered pairs of distinct vertices of G and two weighting functions $\lambda: E(G) \rightarrow \mathbb{R}$ and $w: V(G) \rightarrow \mathbb{R}$ which assign positive real numbers (weights) to edges and vertices, respectively. The weight of a path (cycle) is the sum of the weights of its edges and the weighted degree of a vertex is the sum of the weights of the edges incident with the vertex.

An automorphism of a weighted graph G is a permutation g of the vertex set of G with the following properties:

- For every vertex u and v , $g(u)$ and $g(v)$ are adjacent if and only if u and v are adjacent;
- for every vertex v and edge e , $w(g(v)) = w(v)$ and $\lambda(g(e)) = \lambda(e)$.

The set of all automorphisms of a graph G , with the operation of composition of permutations, is a permutation group on $V(G)$, denoted $\text{Aut}(G)$. This group is called the automorphism group symmetry of G . This group does not fully determine molecular geometry, but it represents the maximal symmetry which the geometrical realization of a given topological structure may possess.

In this talk, we report our recent results on computing the symmetry of some cubic molecules containing generalized fullerenes. Some methods for computing the symmetry-based graph invariants are also presented.



On Graovac-Pisanski index of polyhedral graphs

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Abstract. The Graovac-Pisanski index proposed in 1991 for generalizing the Wiener index by means of automorphism group of considered graph. In this paper, we compute the difference between these topological indices for a class of polyhedral graphs.

1. Introduction

All graphs considered in this paper are connected and simple. Let Γ is a graph with vertex and edge sets $V(\Gamma)$ and $E(\Gamma)$, respectively. Two vertices u and v are adjacent if $uv \in E(\Gamma)$. The distance $d(x, y)$ between two vertices $x, y \in V(\Gamma)$ is defined as the length of the shortest path between them. A connected graph is one whose all vertices are connected by a path.

Let \mathcal{G} be the class of all connected graphs, a topological index is a function $g: \mathcal{G} \rightarrow \mathbb{R}^+$ which is invariant under the automorphism group of Γ . The Wiener index is defined as the half sum of distances between all pairs of vertices in a molecular graph, see Refs. [1,2].

Assume that Γ is a graph with automorphism group $G = \text{Aut}(\Gamma)$, then the Graovac-Pisanski index is defined as

$$\hat{W}(\Gamma) = \frac{|V(\Gamma)|}{2|G|} \sum_{x \in V(\Gamma)} \sum_{\alpha \in G} d(x, \alpha(x)). \quad (1)$$

Theorem 1 [3]. Let Γ is a graph on n vertices. Let V_1, V_2, \dots, V_k be all orbits of action $\text{Aut}(\Gamma)$ on the set of vertices. Then

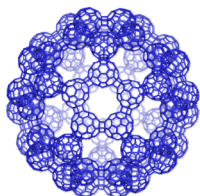
$$\hat{W}(\Gamma) = n \sum_{i=1}^k \frac{W(V_i)}{|V_i|}. \quad (2)$$

For given graph Γ the difference between Wiener and modified Wiener indices is defined by Hakimi-Nezhaad et al. [4] as $\delta(\Gamma) = W(\Gamma) - \hat{W}(\Gamma)$.

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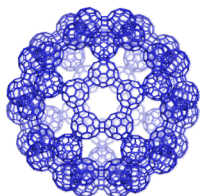


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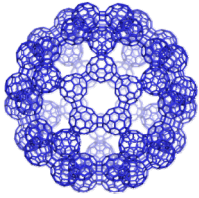
GEOMETRY OPTIMIZATION OF nC_{24} CYCLIC POLYIYNE CLUSTER

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Background. In a previous study were investigated the optimal size of polyynes to form rings (and was found to be 24) as well were investigated the conformation of a cluster of 4 crossing C_{24} cyclic polyynes. Geometry optimization of molecular clusters is slightly different than the geometry optimization of molecules since at clusters the degrees of freedom no longer represents the atoms positions itself but the molecules positions. **Aim.** Here are reported a study regarding the developing of an geometry optimization (energy minimization) program at molecular mechanics theory level designed to provide a good profile for the conformation of crossed nC_{24} polyynes by the pattern previously found - each cyclic polyiyne is crossed by another 3. **Material.** Clusters of nC_{24} were designed by the pattern by involving successive geometrical 3D rotations and translations and replications of the C_{24} cyclic polyiyne as well as of its cluster. The resulted cluster was subjected to energy minimization and a program was developed to do this. **Method and algorithm.** Several tricks were found and implemented during the program development. A molecule (C_{24}) position was characterized by its center (three Cartesian coordinates) and its direction (three angular coordinates). Thus, the subject of optimization was $6 \cdot n$ variables corresponding to the degrees of freedom of the molecules positions in the cluster. Since all atoms are Carbon, and all atoms have the same constrains (a single and a triple bond) supplementary coefficients or constants other than the distance parameterizing interaction were not necessary. The optimization objective which was found to be suitable is the sum of the inverses of the fourth power of the distance between atoms to minimum. Other trick is how to keep the molecules together since the tendency of the optimization score is to depart the molecules one to any other. **Program and results.** A FreePascal program was developed and parameterized correspondingly to be used for any value of the n to do the geometrical optimization of the nC_{24} cluster. Program has been tested for $n = 4$, $n = 10$ and $n = 22$ and it works. In order to keep the molecules together, a module identifying the crosses was developed and used as constrain during the optimization. The crosses of each molecule to another are actually the second topology level of the cluster, if the bonds between the atoms are considered to be the first. **Conclusion.** The study revealed that the developed program performs very well in the optimization of the geometry of the cluster.

Keywords: Software for cluster modeling; Cyclic polyiyne clusters; Geometry optimization (energy minimization)



Diamond and diamond-like carbon films: a brief review

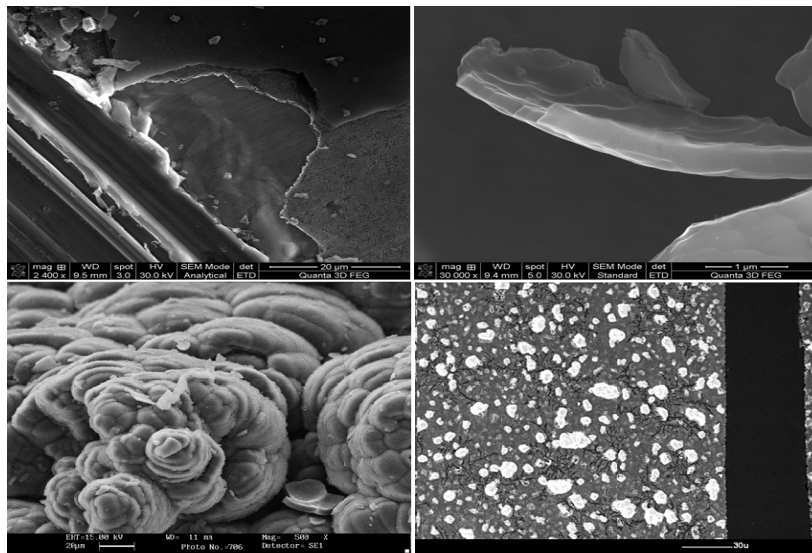
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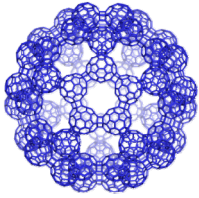
Carbon is one of the most important natural elements, shows several allotropes, such as carbon nanotubes, carbon nanowalls, diamond and diamond-like carbon, etc. Among different hybridizations, two of the most important are diamond and diamond like carbon (DLC). The sp^3 form is involved in diamond structure. However, an amorphous phase containing from less than 1 at% to about 50 at% hydrogen is formed as DLC. Due to the percentage of the sp^n ($n=1, 2, 3$) fraction in its structure, one can divide it to many groups, giving them attractive physical and mechanical properties, some similar to a certain extent to diamond. By developing the Chemical Vapor Deposition (CVD) methods, the deposition of these structures by various CVD techniques has become a favorite topic of by wide research. In this work, a brief review of diamond and DLC production and application our research group since 2010-2017 were investigated.

Keyword: Diamond, DLC, Doping, CVD methods.



TYPICAL FIGURE. SEM images of the deposited Diamond and DLC using CVD system

1. G.V. Zhizhin, Z. Khalaj, M.V. Diudea, Distance, Symmetry, and Topology in Carbon Nanomaterials, Springer, Carbon Materials: Chemistry and Physics (vol.9), 2016



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Molecular dynamics simulation of carbon structures inside nano chambers

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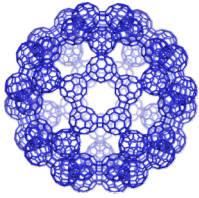
Based on recent experimental results of hydrocarbon formation in small diameter carbon nanotubes filled with ferrocene molecules [1,2], we have performed molecular dynamics calculations. We put 60, 80, 84, 85, 90 and 100 number of carbon atoms in a (14,0) nanotube of length 25.578 Å. In the initial position the carbon atoms were set in C₅ rings and during the simulation the positions of the nanotube atoms were fixed. The carbon-carbon interactions inside the tube were calculated with a density functional adjusted tight binding method, whereas the carbon-carbon interaction with the nanotube was taken into account with a Girifalco-potential. The temperature inside the nanotube was controlled by a Nosé-Hoover thermostat and periodic boundary condition was applied in the model. We have found that the structures formed during the simulation depend on the temperature, the density of the carbon atoms and in some test calculations we have found dependency on the tube diameter as well. At lower temperatures we obtained graphene ribbons and at higher temperature nanotube or fullerene were obtained depending on the density of the carbon atoms. In order to test our results on larger systems, including also hydrogen atoms, molecular dynamics calculations are in progress using the open source code LAMMPS.

Support from OTKA in Hungary (Grant No. K115608).

Keywords: *molecular dynamics, nanoribbons, fullerenes, carbon nanotubes*

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On the eigenvalues of fullerenes

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Abstract. The concept of energy of graph is defined in 1978 by Gutman as the sum of the absolute values of the eigenvalues of a graph. Let $\lambda_1, \lambda_2, \dots, \lambda_n$ be eigenvalues of graph G , then the energy of G is defined as $E(G) = \sum_{i=1}^n |\lambda_i|$. The aim of this article is to estimate the energy of small fullerenes and then we compute some bounds for big fullerenes.

Keywords: eigenvalue, fullerene, graph energy.

1. Introduction

A **fullerene** is a planar three connected cubic regular graphs with pentagonal and hexagonal faces satisfying in Euler's formula. The first and most stable fullerene is C_{60} a fullerene with exactly 60 carbon atoms.

By using Euler's theorem, one can easily prove that a fullerene on n vertices has exactly 12 pentagones and $n/2 - 10$ hexagones where n is a natural number equal or greater than 20 and $n \neq 22$, for more details about mathematics of fullerene graphs see Refs [3-11].

Now we recall some algebraic definitions that will be used in this paper. Throughout this paper, our notation is standard and mainly taken from [12-15]. Let G be a simple molecular graph namely a graph without directed and multiple edges and without loops. The vertex and edge-sets of G are represented by $V(G)$ and $E(G)$, respectively. The adjacency matrix $A(G)$ of graph G with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ is the $n \times n$ symmetric matrix $[a_{ij}]$ such that $a_{ij} = 1$ if v_i and v_j are adjacent and 0, otherwise. The characteristic polynomial $\chi(G, \lambda)$ of graph G is defined as

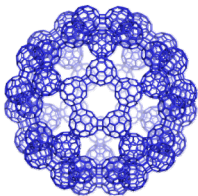
$$\chi(G, \lambda) = \det(A(G) - \lambda I).$$

The roots of this polynomial are eigenvalues of G and form the spectrum of graph as follows:

$$\text{Spec}(G) = \begin{pmatrix} \lambda_1 & \lambda_2 & \cdots & \lambda_n \\ m_1 & m_2 & \cdots & m_n \end{pmatrix}$$

where m_i is the multiplicity of eigenvalue λ_i .

*Author to whom correspondence should be addressed (E-mail: mghorbani@srttu.edu).



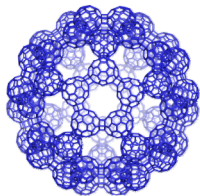
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If G is a graph on n vertices and $\lambda_1, \lambda_2, \dots, \lambda_n$ are the eigenvalues of its adjacency matrix, then the energy of G are defined as [16]:

$$E(G) = \sum_{i=1}^n |\lambda_i|.$$

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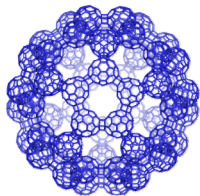
ON THE HARMONIC INDEX AND HARMONIC POLYNOMIAL OF CORCOR DOMAIN OF GRAPHENE

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The harmonic index is one of the most important indices in chemical and mathematical fields. It's a variant of the Randić index which is the most successful molecular descriptor in structure-property and structure activity relationships studies. The harmonic index gives somewhat better correlations with physical and chemical properties comparing with the well-known Randić index. Harmonic index $H(G)$, of a graph G is defined as the sum of weights $\frac{2}{d(u) + d(v)}$ of all edges in $E(G)$, where $d(u)$ denotes the degree of a vertex u in $V(G)$. The harmonic polynomial of G is defined as $H(G, x) = \sum_{uv \in E(G)} 2x^{d(u)+d(v)-1}$, where $\int_0^1 H(G, x) dx = H(G)$. We present here explicit formulas for the values of harmonic polynomial and harmonic index of the molecular graph of a new type of graphene named CorCor that is a 2-dimensional carbon network.

Keywords: Harmonic index, Harmonic polynomial, Randić index



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Hemoglobin versus hemerythrin - based blood substitutes

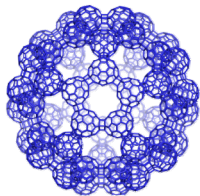
Florina Scurtu^a, Cristina Bischin^a, Cristina Gruian^a, Anca Farcaș^a, Vlad Toma^a, Radu Silaghi-Dumitrescu^{a*}

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We have previously reported an evaluation of a range of physiological parameters in rats injected with small amounts of blood substitute candidates based on hemoglobin. These candidates are mostly nano-sized polycondensates/polymers, as shown by chromatographic and spectroscopic measurements. Generally, they displayed distinctly varying prooxidative reactivity both in vitro and in vivo. Our hypothesis was that less prooxidant Hb derivatives/polymers will display less negative pathophysiological effects. All candidates appeared to behave very similarly to each other in terms of biochemical and immunological parameters, although the less redox-reactive ones were found to lead to less excessive accumulation of iron in organs, and lower amounts of excess paramagnetic species in blood. Here, the comparison is extended to a range of hemerythrin-based preparations. These include copolymers with albumin and with rubrerythrin as redox-protective agents, characterized in terms of size, reactivity and stability. The hemerythrin-based candidates are shown to elicit in rats physiological parameters remarkably similar to those elicited by hemoglobin-based polycondensates. Preliminary data on the effect of such blood substitute candidates in hemorrhagic shock induced in Wistar rats will also be discussed.[1,2]

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Theoretical investigations regarding the properties and applications of fullerenes and their precursors

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The large number of applications of fullerenes that have emerged within the last years have attracted a continuous interest for their investigations^{1,2}. Taking into account that the unique properties of the fullerenes are mainly due to their extended π electron system, the first goal of the study consists in the evaluation of the aromaticity of the precursors of these nanomaterials. In this regard, various geometric, magnetic and electronic descriptors like HOMA (Harmonic Oscillator Model of Aromaticity), NICS (Nuclear Independent Chemical Shift), ELF (Electron Localization Function) have been computed; also, as a measure of reactivity in the electrophilic substitution reaction, the Fukui functions for an electrophilic attack have been calculated.

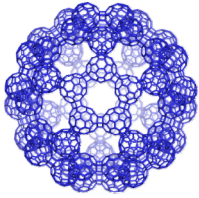
A possible way to influence the extended π -electron systems is to introduce one (or more) heteroatom. As a result, the second goal of the study was to establish the variation of the properties of the hetero-compounds. Investigations regarding both geometry and properties changes and comparisons to the all-carbon compounds have been performed.

Using the studied circulenes as repeating units, hypothetical fullerene structures have been built and computations regarding their properties and stability have been performed. On the basis of the obtained results, the connections between the properties of the fullerenes and the properties of the circulenes pattern have been established.

Also, studies regarding the possible applications of the investigated fullerenes in the medical field, consisting in the analysis of their interactions with biologic active compounds have been performed.

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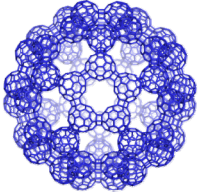
Toxicity Assessment and Regulation of NanoHealth Products in Iran: Effectiveness and Challenges

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Engineered nanomaterials (ENMs) have gained considerable interests during last decade due to their excellent health activities. Despite their extensive use, the potential safety of ENMs and possible mechanisms by which they may induce adverse reactions have not received sufficient attention and no specific knowledge translations exists in a practical model to describe and quantify their toxic effects for their regulation, standardization and clinical applications. ENMs don't undergo routine biotransformation pathways therefore their biological fate and half-life could not be determined well however they may interfere with biotransformation of pharmaceuticals which may cause drug overdosing or underdosing, with harmful and even life-threatening consequences for patients. Other parameters, such as surface/volume ratio, chemical stability, and tendency to aggregation can result in reactivity of ENMs with critical genes and proteins in target organs. Although we are not able, at present, to identify all possible toxic effects of registered Nanohealth products, we used a battery of toxicology tests using cellular and animal models as well as clinical settings to predict local and systemic effects of ENMs by focusing on their genotoxic potentials, target organ toxicities and Adverse Drug Reactions respectively. We tried in our 8 years efforts to provide an opportunity for clinical application of more than 70 Nanohealth products in the market of Iran by developing great toxicological models but there are still lack of knowledge translation for many classes of ENMs to provide realistic health risk assessment and management.

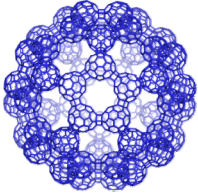


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Constructions of graphs and trees with partially prescribed spectrum

Xueliang Li

It is shown how a connected graph and a tree with partially prescribed spectrum can be constructed. These constructions are based on a result of Salez that every totally real algebraic integer is an eigenvalue of a tree. Our result implies that for any (not necessarily connected) graph, there is a tree such that the characteristic polynomial of the graph divides the characteristic polynomial of the tree. Some open problems will also be presented in this talk. This is a joint work with Ivan Gutman and Wasin So.



Investigating the Physical Properties of ZnFe_2O_4 Nanocrystals synthesized by Co-Precipitation Method

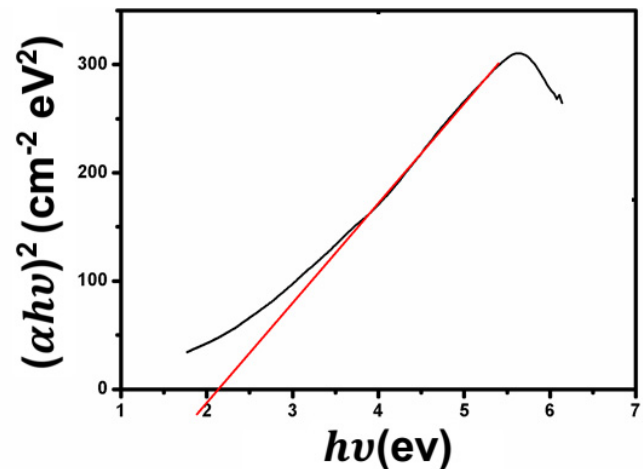
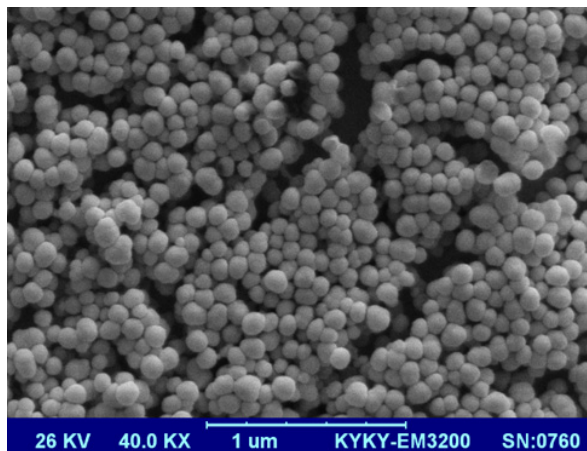
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Zinc Ferrite (ZnFe_2O_4) nanoparticles with diameter less than 100nm were successfully synthesized with co-precipitation method. All the samples were annealed at 500°C, 600°C and 700°C in furnace for one hour. The structure, morphology and physical properties of the samples were characterized by means of powder X-ray diffraction (XRD), scanning electron microscopy (SEM) and UV-Visible transmission spectroscopy. The results show a good crystalline structures with different crystallinity. The optical properties were studied by recording the transmittance and absorbance spectra in the range of (200 - 700) nm. The optical band gap energy of ZnFe_2O_4 powders were estimated at different annealing temperatures by Tauc's method which was measured about 2.13eV.

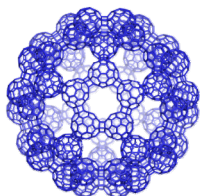
Keyword: ZnFe_2O_4 nanoparticles, XRD, Optical gap



TYPICAL FIGURE. SEM images and Energy gap diagram of ZnFe_2O_4 after thermal annealing in 500°C.

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A categorical approach to chemical reactions

Andres Bernal¹, Wilmer Leal², Eugenio Llanos³, and Guillermo Restrepo⁴

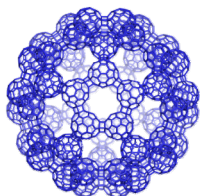
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Historically, similarities among chemical reactions led to classification of substances, e.g. amines and acids, to name but a few classes. However, the focus on the relational character of reactions was abandoned and changed for the resemblance among properties of bulk substances and later on for the similarity of molecular structures. Here we show that the original chemical similarity based on reactions can be formalised using elements of category theory, where substances are characterised by their relations. Category theory is the mathematical framework where objects are determined by their viable transformations, which is as we understand chemical reactions. As a category is made by a collection of objects and another of morphisms, the objects in this approach are graphs and the morphisms relations between graphs, $r : G \rightarrow G'$, where G is the network of chemical reactions and G' is the resulting graph of classes of chemical substances. We found that r denotes a formal context of Formal Concept Analysis (FCA), bringing the appropriate framework to look for well-defined classes of similar substances. These classes correspond to concepts in FCA, which are derived using a closure operator. The methodology is applied to the decomposition reactions of a set of more than 7,000 binary compounds, which allows obtaining a classification for chemical elements, where traditional and new families of elements are found. Our results indicate that the categorical approach to chemical reactions, besides formalising the concept of chemical similarity, can be used to treat the whole network of chemical reactions and to explore the current status of chemical classes.



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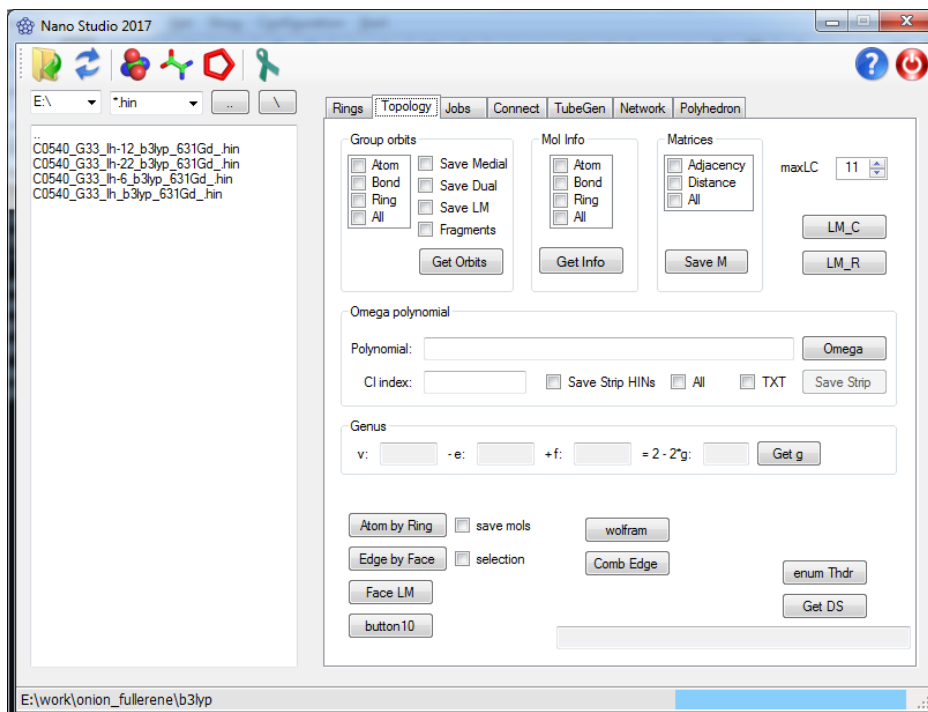
The Nano Studio software

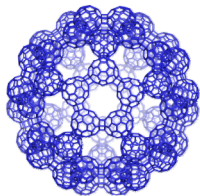
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The Nano Studio software was designed for the generation or further modification of the geometry of carbon nanostructures, including nanotubes, fullerenes, or multiterminale nanotube junctions. The program was developed in Visual C# and requires the Microsoft .Net Framework to be installed. It includes several tools for the topological characterization of structures, including the classification of atoms, bonds, and rings by orbits. It allows the topological transformation of a structure using the dual, medial, leapfrog, and other map operations.

The program works with the HyperChem chemical file format, and requires the molecule to be saved as HIN file. The figure below shows a screenshot of the topology tab of the program.





Water solvation clusters in assessing polymers toxicity

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Poliethylenimine (PEI) and polyamidoamine (PAMAM) are used widely in fields such as biochemistry, biotechnology, nanotechnology. These molecules, by i.v. administration come in contact with biological systems or with whole organisms. Their ADME properties, toxicity and reactivity are widely tested. Such molecules are subjects of functionalization and derivatization. Toxicity and reactivity of congeneric compounds can be determined by computational methods such as QSAR. In this study, QSAR and virtual high throughput toxicity screeningⁱ (vHTS) based toxicity methods are applied on some (novel) synthesized zero, first and aromatic core dendrimersⁱⁱ generation to evaluate their toxicity. Two predictive models were computed:(i) a model that compute the probability of interaction; (ii) a model that computes the toxicity values in terms of spectral values assessing viability of culture cells. Toxicity evaluation was performed experimentallyⁱⁱⁱ. Prediction models were used to predict toxicities for related generation dendrimers.

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