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Effects of Electromagnetic Fields on Human Serum Paraoxonase-1 Activity in Vitro

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In recent years the relationship between electromagnetic fields and coronary artery disease is attracted a considerable attention. Low density lipoprotein (LDL) oxidation is the initial step in the development of atherosclerosis. Paraoxonase1 (PON1) protects LDL and High density lipoprotein (HDL) against oxidative processes, thus preventing the formation of atherogenic ox-LDL molecules. In this study we investigate the effects of extremely low frequency electromagnetic fields (ELF-EMFs) on PON1 activity as one of the independent risk factors for cardiovascular disease. Pooled serum sample of 20 healthy men were exposed to electromagnetic flux density of 0.125, 0.25, 0.5, 1, 2, 3 and 4 mT for 60, 120 and 180 minutes at 25°C and then PON1 activity was measured spectrophotometrically using paraxon as substrate. EMFs of 0.125- 1 mT have no effect on PON1 activity. Exposure to magnetic flux density of 2 mT leads to a significant increase in PON1 activity in 2 hours. Magnetic flux density of 3 and 4 mT lead to an increase in PON1 activity to 1.2% and 2.8% after 1 h of exposure respectively. PON1 activity is influenced by a variety of agents like environmental, pharmacological, and lifestyle factors as well as age and sex. According to the finding of this study ELF-EMFs can alternate the serum activity of PON1 in vitro. If this effect of EMFs on PON1 activity has proven in vivo, it can be considered as an effective factor in coronary artery disease.

Keywords: *Paraoxonase-1, Electromagnetic fields, coronary artery disease*

DFT Benchmarking for the Correct Description of Spin States in Bioinorganic Centers. Heme vs. Siroheme Models of the Sulfite Reductase Active Site

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ABSTRACT. A test set of models that describe bioinorganic centers was employed to benchmark the performance of several density functional methods for the accurate description of overall spin states of these centers. The set comprises four models derived from biological active sites that possess different ground state multiplicities (high-spin, low-spin and intermediate-spin state), as depicted in Figure 1.

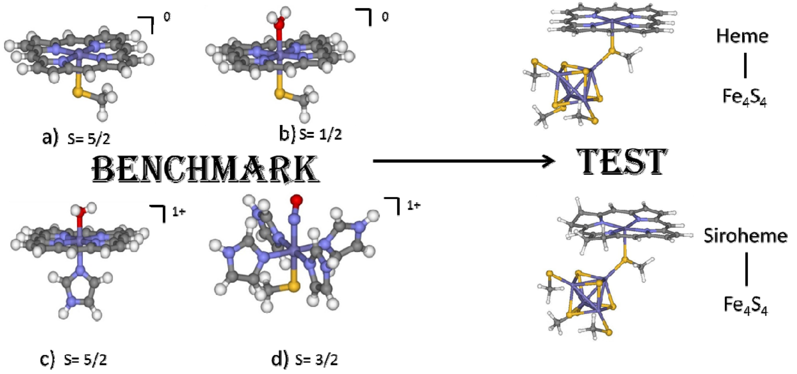

Fig.1. Left: Bioinorganic models derived from the active sites of: ferric cytochrome P450 with a vacant distal position (a) and aqua-bound (b), ferric hemoglobin (c) and ferrous-nitrosyl superoxide reductase (d). Right: Heme-[Fe4S4] and Siroheme-[Fe4S4] systems

A set of functionals that use a different amount of exact Hartree-Fock exchange in their evaluation of the exchange integrals was tested. Further theoretical investigations are carried out with the best performing functionals on bioinorganic models derived from the active site of sulfite reductase in which differences in terms of energetics, bonding, spin coupling are emphasized between the biologically occurring siroheme-[Fe_4S_4] system and the fictive heme-[Fe_4S_4] system in order to give more insights on nature's preferences for the former system over the latter.[1,2]

REFERENCES

1. M. Surducan,D. Lup,A. Lupan,S. V. Makarov,R. Silaghi-Dumitrescu, *Journal of Inorganic Biochemistry*, **2013**, *118*, 13-20
2. M. Surducan,S. V. Makarov,R. Silaghi-Dumitrescu, *European Journal of Inorganic Chemistry*, **2014**, *34*, 5827-5837

On the Laser Ablation Capability to Synthesyse Nanostructures

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Numerous techniques have been used to synthesize nanostructures. Among them, pulsed laser ablation (PLA) method has become a significant technology to produce nanostructures. This technique has many major advantages compared to other techniques, like; inexpensive equipment to control the ablation atmosphere, the simplicity of the experimental setup and the ability to control the morphology of synthesized material by changing different parameters such as laser wavelength, laser pulse duration, laser fluence, the pH of the solution, solution temperature, and so on. Furthermore PLA is an environment-friendly technique since there will not be any by-products after production of nanostructures.

In this experimental investigation, effects of several parameters of laser pulse on the morphology of graphene nanosheets produced by PLA method has been reported. Graphene nanosheets were produced by irradiation of graphite target. Several techniques such as TEM and SEM imaging, UV-Vis-NIR, FTIR, and Raman spectroscopy were employed to study the features of produced nanosheets. Results show that PLA is a capable mechanism to produce nanostructures [1-2].

Keywords: *pulsed laser ablation; graphite; graphene*

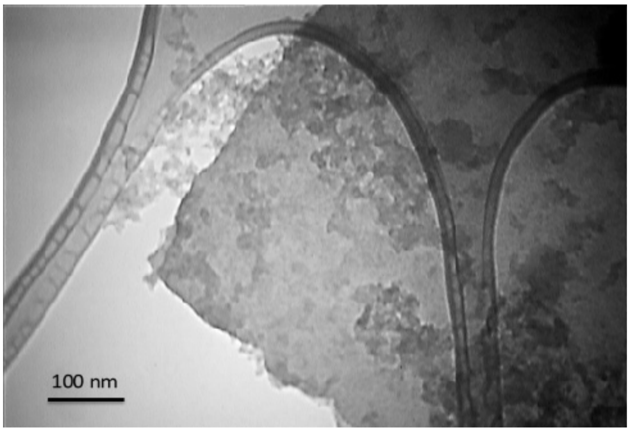

Fig. TEM image of a graphene nanosheet and carbonic nanoparticles.

REFERENCES

1. E. Solati, D. Dorranian, *Appl. Phys. B*, **2016**, *76*, 122.
2. N. Tabatabaie, D. Dorranian, *Appl. Phys. A*, **2016**, *122*, 558.

Predicting Gap Energy and Ionization Energy of Oligorylenes Family Based on TIM

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ABSTRACT. Homologous classes of Polycyclic Aromatic Hydrocarbons has numerous applications in materials science and technology. One classes of PAHs is Oligorylenes. A topological index (also known as molecular descriptor) is any function on a graph that does not depend on a labeling of its vertices.

In this paper, we will increase the physico-chemical applicability of the topological index. First of all, the explicit formula of Hyper zagreb index of Oligorylenes family is computed and various models to predict some thermodynamic properties including Ionization Energy and Gap Energy is presented. Finally, all models are examined for some heavier members of Oligorylenes family.

All information about the first members of Oligorylenes family were derived from reliable experimental data and valid references.

Keywords: *Oligorylenes, Gap Energy, Ionization Energy, Hyper zagreb index.*

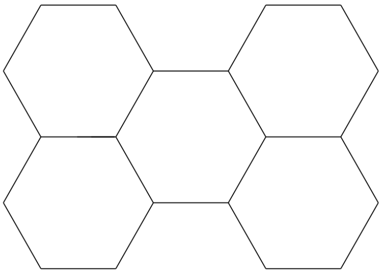

Figure. chemical molecular graph of perylene

REFERENCES

1. G. Malloci, G. Mulas, G. Cappellini, C. Joblin, Chemical Physics, 340 (2007) 43-58.
2. G. H. Shirdel, H. Rezapour and A. M. Sayadi, The hyper-Zagreb index of graph operations, Iranian J. Math. Chem., 4(2) (2013) 213-220.

Enhanced Photocatalytic Activity of Pb and Co Doped ZnO Thin Films Prepared by Sol-Gel Procedure for Methylene Blue Degradation

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Pb and Co-doped ZnO nanostructure thin films coated on glass substrate by sol gel method for the first time and thin films are characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM) and UV-visible absorption spectroscopy. The all thin films have a polycrystalline hexagonal wurtzite structure and wrinkle morphology. The photocatalytic activity of the prepared thin films were evaluated for degradation of Methylene Blue (MB) solution. The results indicated that Pb dpoing increased the photocatalytic activity of ZnO thin films and Co doping reduced the photocatalytic activity of ZnO thin films.

Keywords: *Pb doping, Co doping, ZnO, Photocatalyst.*

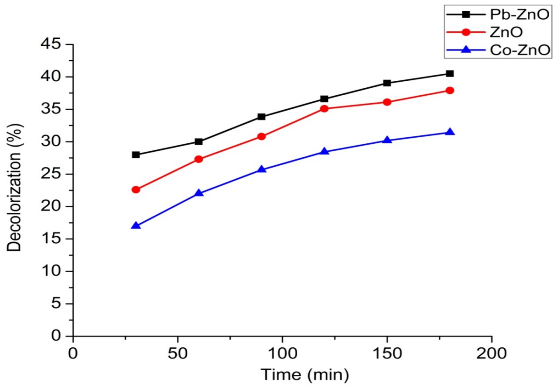

Fig. 1 Time dependence of the decolorization efficiency of MB solution by doped and undoped ZnO thin films.

1.I. Balti, A. Mezni, A. Dakhlaoui-Omrani, P. Leone, B. Viana, O. Brinza, L.S. Smiri, N. Jouini, "Comparative study of Ni-and Co-substituted ZnO nanoparticles: synthesis, optical and magnetic properties", Journal of Physical Chemistry, **2011**, 115: 15758-15766.

Synthesis and Characterization of Kappa-Carrageenan/ Chitosan Coated Cobalt Ferrite Nanocomposite and the Study of Its Swelling Behaviour

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Using polymer-based nanocomposites, especially those consist of natural polymers have become a very popular approach in the biomedical applications like drug delivery, owing to its biocompatibility and biodegradability. The aim of the present work is to synthesize a hydrogel nanocomposite using κ-carrageenan/chitosan and cobalt ferrite magnetic nanoparticle. The magnetic nanoparticle of cobalt ferrite was synthesized in the presence of κ-carrageenan by co-precipitation of iron and cobalt ions through an in-situ method. Magnetic κ-carrageenan was cross-linked by the polycation chitosan biopolymer. The structural characteristics of the hydrogel nanocomposite were evaluated by FTIR, XRD, SEM and VSM techniques. FTIR analysis showed the presence of two above mentioned biopolymers in the composite. The morphology and crystal structure of magnetic nanocomposite were obtained by scanning electron microscopy (SEM) and XRD. Results confirmed the inverse spinal structure of CoFe2O4. The swelling capacity of the hydrogel was also obtained in the current study. The result showed a highly swelling capacity at an aqueous solution where the percentage of swelling ratio for non-magnetic hydrogels was 540 and the magnetic sample was 304. It was found that the degree of swelling of the nanocomposite was decreased by incorporation of magnetic nanoparticles. Also increasing the amount of chitosan decreases the water uptake in the samples.

Keywords: *Magnetic nanocomposite, k-carrageenan, Chitosan, Cobalt ferrite.*

REFERENCE

1. E.M. Ahmed, Hydrogel" Preparation, characterization, and applications: A review", Journal of advanced research, **2015,** 6: 105-121.

Gauge Symmetries in Constrained Systems

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Gauge Theories provide the most significant concepts in theoretical physics as the theoretical foundation for the standard model of elementary particles. The heart of any gauge theory is the gauge symmetry group and the central role that it plays in determining the dynamics of the theory. The crucial difference in gauge theory is that the symmetry group is not associated with any physical coordinate transformation in space-time, rather it is based on an "internal" symmetry. Gauge invariance is due to the presence of the important physical variables which are independent of the local reference frames [1,2]. These identities between phase-space coordinates are classified into two main groups [3,4,5]. The first group is identities which transform the physical system without any changes in the phase-space, and are called first-class constraints. The second group are related to nonphysical degrees of freedom, which are called second-class constraints and indicate the absence of the gauge symmetry in the system. Therefore, gauge symmetry can be studied within the framework of the Hamiltonian formalism for constrained dynamical systems. First-class constraints are considered to be the generators of the gauge transformations in the phase-space. Also, to make a gauge system containing second-class constraints, one should transform them to first-class ones [6, 7]. To do that, there has been existed some approaches such as BFT [8, 9,10], and symplectic formalisms [11, 7] which are based on the fact that the nongauged system will be embedded in an extended phase space, in order to convert the second class nature of constraints into first class ones. It is very important to know that the equations of motion of the original system and the original system obtained via embedding method are equivalent.

[1] M. Henneaux, C. Teiltelboim, Quantization of Gauge System, University Press, (1992). [2] G. 't Hooft, M. Veltman, Nucl. Phys. B 44, 189, (1972). [3] S. Abarghouei Nejad, M. Dehghani, M. Monemzadeh, arXiv: 1508.01866, (2015).
[4] P.G. Bergmann, I. Goldberg, Phys. Rev. 98, 531 (1955). [5] P.A.M. Dirac, "Lectures on Quantum Mechanics", Belfer graduate School, Yeshiva, Univ. Press, New York, (1964). [6] P.A.M. Dirac, "Generalized Hamiltonian dynamics", Can. J. Math.2, (1950). [7] M. Monemzde, M. Dehghani, S. Abarghouei Nejad, Int. J. Theor. Phys. 56, 6 (2017). [8] I.A. Batalin, E.S. Fradkin, Nucl. Phys. B 279, (1987). [9] A. Shirzad, M. Monemzadeh, Phys. Rev. D 72, (2005), arXiv:hep-th/0401230. [10] F. Sarvi, M. Monemzadeh, S. Abarghouei Nejad, Adv. High Energy Phys. 2016, 4638596, (2016). [11] L. Faddeev, R. Jackiw, Phys. Rev. Lett. 60, 1692, (1988).

Growth of $ZnFe_2O_4$ Nanocrystals by Co-Precipitation Method

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Zinc ferrite have been produced and by humans since many years ago, however understanding the nano structure products of $ZnFe_2O_4$ is very useful in order to be used for technological applications. In this work, Zinc ferrites prepared by co-precipitation method using the Zinc oxide ($ZnCl_2$) and Iron (III) chloride hexahydrate ($FeCl_3.6H_2O$). After initial synthesis, the obtained powders put in different beaker and were heated for 3 hours at 100 ˚C in the oven. Afterwards, for annealing treatment, the powder was located in furnace and were heated at 500˚C for one hour. X-Ray diffraction and scanning electron microscopy (SEM) methods were used to characterize the samples. The results show that thermal annealing has a great effect on formation of high crystalline quality of zinc ferrite nanoparticles.

Keywords: *Zinc Ferrite, Thermal annealing, co-precipitation method.*

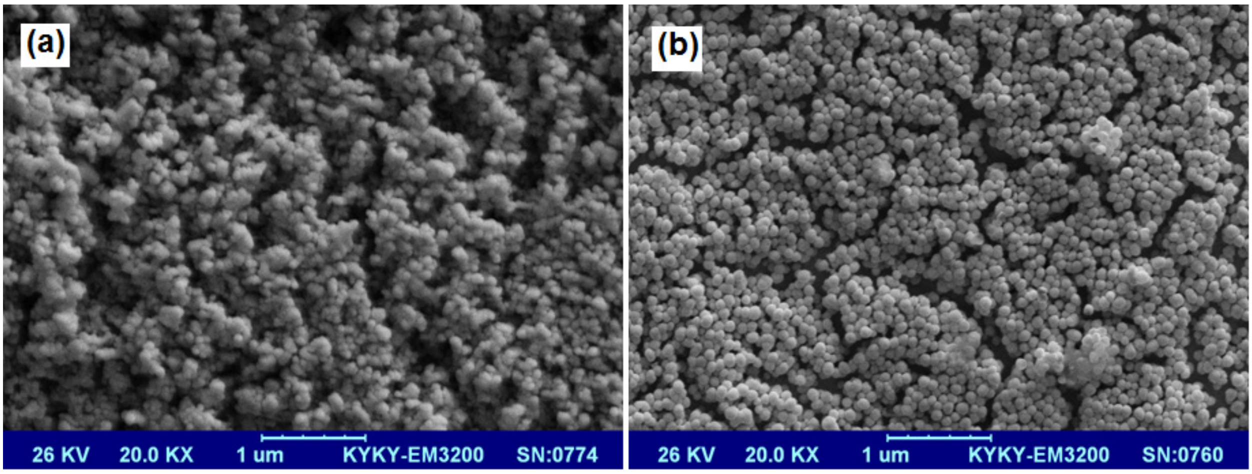

FIG. 1 SEM images of $ZnFe_2O_4$ nanoparticles (a) before annealing (b) after annealing

REFERENCES

1. J. Mayekar, V. Dhar, S. Radha, Synthesis, Characterization and Magnetic Study of Zinc Ferrite Nanoparticle, *International Journal of Innovative Research in Science*, **2016**, Vol. 5, Issue 5, 8367-8371.

Bonding of Carbonyl Groups to the Dipentalene Dititanium System Relating to Products Obtained from CO_2 Activation

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The pentalene dianion $[C_8H_6]^{2-}$ (Pn^{2-}) exhibits a variety of coordination modes, of interest being the ability to form bis-pentalene complexes – where two metals are located between pentalene ligands (the so-called “double sandwich” complexes). The structure of dipentalene dititanium, Pn_2Ti_2 is relatively open so the titanium orbitals are accessible to small molecules. Therefore, dipentalene dititanium in presence of one or two equivalents of CO affords mono- and dicarbonyl compounds [1, 2]. With excess of CO, the tri-carbonyl complex is generated [3].

We have performed DFT calculations on $Pn_2Ti_2(CO)_n$ systems, where n = 1 – 4. The experimentally reported structures are shown to be the global minima for these systems.

Keywords: *pentalene, DFT, carbonyl*

REFERENCES

1. A. F. R. Kilpatrick, J. C. Green, F. G. N. Cloke, *Organometallics*, **2015**, *34*, 4830.
2. A. F. R. Kilpatrick, J. C. Green, F. G. N. Cloke, *Organometallics*, **2015**, *34*, 4816.
3. A. F. R. Kilpatrick, F. G. N. Cloke, *Chem. Commun*, **2014**, *50*, 2769.

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CALCULATING DIFFERENT TOPOLOGICAL INDICES OF IDEMPOTENT GRAPH OF Z_n

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Let R be a ring with identity. By $Id(R)$, we mean the set of all idempotents of R. In [2], $G_{Id}(R)$ is a graph with vertices of R such that two vertices u and v are adjacent if and only if $u \mid v \subset Id(R)$. Let $R = \mathbb{Z}_n$ such that $n = p_1 \times \dots \times p_k$ be a positive integer where for $1 \leq i \leq k$, p_i's are distinct prime numbers such that $p_1 < \cdots < p_k$. Let $|Id(\mathbb{Z}_n)| = m$, for some positive integer m and d_u is the degree of vertex u. If $2u \in Id(R)$, then $d_u = m - 1$. If $2u \notin Id(R)$, then $d_u = m$. For given rings R and S, if $R \simeq S$, then $G_{Id}(R) \cong G_{Id}(S)$ as graphs. The example is shown in figure1. For the edges set $E(G_{Id}(R))$, we have

$$|E(G_{Id}(R))| = \begin{cases} n-1 & If\ n = {p_1}^{\alpha_1} \\ \frac{n(m-1)}{2} & If\ n \neq {p_1}^{\alpha_1}\ and\ n\ is\ even \\ \frac{(n-1)m}{2} & If\ n \neq {p_1}^{\alpha_1}\ and\ n\ is\ even \end{cases}$$

The Zagreb indices are $M_1(G) = \sum_{u \in V(G)} (d_u)^2$ and $M_2(G) = \sum_{u,v \in E(G)} d_u d_v$.

The Randić index of a graph G is defined such as $\chi(G) = \sum_{u,v \in E(G)} \frac{1}{\sqrt{d_u d_v}}$. The other indices are $GA(G) = \sum_{u,v \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u d_v}$ and $ABC(G) = \sum_{u,v \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$. In this paper, we compute all of the indices of $G_{Id}(R)$ mentioned above.

Keywords: *Idempotent graph; the first Zagreb index; the second Zagreb index; Randić index.*

Figure1. The Idempotent graphs of two isomorphic rings

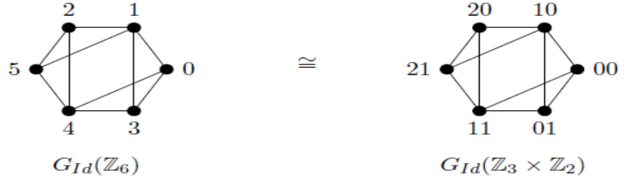

Table1. The value of some indices of Idempotent Graph $G_{Id}(\mathbb{Z}_n)$

n	$M_1(G_{Id}(\mathbb{Z}_n))$	$M_2(G_{Id}(\mathbb{Z}_n))$	$\chi(G_{Id}(\mathbb{Z}_n))$	$GA(G_{Id}(\mathbb{Z}_n))$	$ABC(G_{Id}(\mathbb{Z}_n))$
2	1	1	1	2	0
6	68	114	1.3	5.95	7.03
9	30	28	3.65	12.6	6.42
15	212	400	4.01	11.87	10.66

1. E. Estrada, L.Torres, L. Rodriguez and I. Gutman, An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes,Indian J.Chem., 37A(1998),849-855.

Some Polyhedral Graphs Of Bionanotechnology Interest

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A retracting-free bidirectional circuit in a graph G is a closed walk which traverses every edge exactly once in each direction and such that no edge is succeeded by the same edge in the opposite direction. Studying the class of all graphs admitting at least one retracting-free bidirectional circuit was proposed by Ore (1951) and is, by now, of practical use to nanotechnology. The last needs in various molecular polyhedra that are constructed from a single chain molecule in the retracting-free way.

A cubic graph Q 2 has 3h edges, where h is an odd number _ 3; thus, in particular, no
15 cubic graph with an even number of edges can belong to . The graph of the triangular prism is the minimum cubic graph Q 2 , having 6 vertices and 9 edges. The minimum polyhedral graph G in has 5 vertices and 8 edges, and corresponds to the square pyramid. We begin to analyze some possibilities for deriving new graphs with an odd number of edges from a graph G 2 using graph-theoretical operations. Such cases include: (1) the dual dua(G) having the same number m of edges as G; (2) the truncation tru(G) and (3) leapfrog lpf(G), each having 3m edges; (4) the snub snb(G), with 5m edges; and (5) the septupling sep(G) having 7m vertices. Each of these operations produces a polyhedron graph under the action on any graph of the polyhedron.

Some other relevant questions are discussed in the main body of the report.

Keywords: cubic (polyhedral) graph, spanning tree, cotree, retracting-free bidirectional double circuit, dual, truncation, leapfrog, polygonal, snub, septupling.

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Cobalt vanadate nanostructures: Size controllable synthesis, characterization and enhanced photocatalytic activity for the degradation of organic dyes

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Semiconductor photocatalyst is one of the most common and useful technologies to reduce or destruction of pollution because it illustrates simple condition to utilize natural or artificial irradiation that is available everywhere. Moreover, material in nano scale show unique properties compared to what they show in micro scale. Catalytic behavior is not only strongly materials-dependent but also extremely size-dependent. Henglein showed that a nanomaterial can exhibit very different behaviors compared to its bulk self. For this purpose, nanomaterials use as photocatalyst due to increasing surface to volume ratio which raise surface energy associated with particles. The various types of photocatalysts are available that most famous of them can be noted TiO_2. But researches continue to replace or improve the properties of the photocatalyst materials. However, wide band gap (3.2 eV) of TiO_2 caused researchers to reduce band gap of photocatalyst material which exposed to visible light for destruction of organic dyes. A series of compounds with low band gap are vanadates such as $BiVO_4$, $FeVO_4$, $AgVO_3$, Ag_3VO_4, $Cu_3V_3O_8$ and $Zn_3V_2O_8$. Cobalt vanadate, as one of the most important family of vanadate materials, have suitable band gap for the destruction of pollutants. There are numerous classes of cobalt vanadates such as $Co_3V_2O_8$, $Co_2V_2O_7$ and CoV_2O_6. Different types of cobalt vanadate nanostructures such as $Co_3V_2O_8$, $Co_2V_2O_7$ and CoV_2O_6 have been successfully prepared via a simple solid-state method. For the first time, cobalt vanadate nanostructures were synthesized via Schiff-base ligand and vanadyl sulfate as a capping agent and vanadium source, respectively. The effect of a Schiff-base ligand (N,N-Bis (salicylaldehyde) ethylenediamine = H_2salen) as a capping agent, molar ratio of Co: H_2salen and Co:V on type of products, morphology and size of cobalt vanadate nanoparticles was investigated to reach optimum condition. The as-prepared nanostructures were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), transmittance electron microscopy (TEM), Fourier transform infrared (FT-IR) spectra, energy dispersive X-ray microanalysis (EDX) and ultraviolet–visible (UV–Vis) spectroscopy. This work is the first study on photocatalytic activity of cobalt vanadate nanostructures in different conditions. The influence of different parameters such as type of cobalt vanadate nanostructures, type of dye, size of particles and nanostructures dosage as a catalyst on photocatalytic activity of samples were studied.

Keywords: Nanostructure; Solid-state; Photocatalytic activity.

NANO-DENDRIMERS IN EARLY STAGES OF CRYSTAL NETWORKS

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Keywords: nano-dendrimer; multi-torus; Hartree-Fock.

Abstract. Polybenzene 6.8^2D was described by O'Keeffe *et al.* (1992) as a uninodal network: *pbz* (space group *Pn*-3*m*, with the *fcc*-diamond topology and point symbol net $\{6.8^2\}$); it is embedded in the infinite periodic minimal *D*-surface and was predicted to be an insulator and having a substantially lower energy per atom in comparison to the reference C_{60} fullerene. Its repeating unit, BTA.48, has an "armchair"-ended structure; it can form three dimers: (i) the dimer 2(BTA.48)[8_{fcc}].88 that further provides the diamond-like *fcc* net 6.8^2D; (ii) an intercalated dimer 2(BTA.48)[12_{int}].84 that further forms dendrimers (Diudea and Katona, 1999; Szefler and Diudea, 2012) and (iii) an eclipsed dimer 2(BTA.48)[12_{ecl}].90 which can further form multi-tori. The number in the right brackets is the size of the "windows" identified when a dimer is formed.

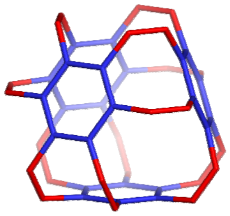
The "intercalated" dimer forms a first generation dendrimer, 5(BTA.48).192 and a second generation dendrimer 17(BTA.48).624 (see the below figure). A further growing of the dendritic net will completely be superposed over the diamond-like network. The "eclipsed"-dimer and its oligomers show angles suitable to form structures of five-fold symmetry, particularly multi-tori (Diudea and Petitjean, 2008; Diudea, 2010).

A polybenzene "zig-zag"-ended unit, BTZ.24 is also known; it forms only two dimers: (a) an eclipsed dimer 2(BTZ.24).48, suitable to rather build multi-tori than dendrimers and (b) a dimer 2(BTZ.24).42 that provides a translational network called *uta* (space group *Fd*-3*m* and point symbol net $\{6.9^3\}$).

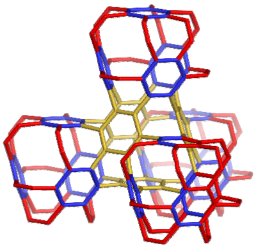
Multi-tori are complex structures including negatively curved units (Diudea, 2010; Diudea and Nagy, 2007); they may result by self-assembly of some monomers, possibly formed by spanning of fullerenes, and can appear in spongy carbon and in natural zeolites as well; they can grow radially (providing spherical shaped structures) or linearly, giving rod-like periodic nets.

The energetics of monomers, dimers and some small substructures of polybenzenes were evaluated at the Hartree-Fock (6-31G**) level of theory. In the hope of their future experimental synthesis, vibrational spectra of the most important monomers and dimers were simulated (Szefler *et al*. 2012). Topology was evaluated in terms of ring signature index RSI (Nagy and Diudea, 2017).

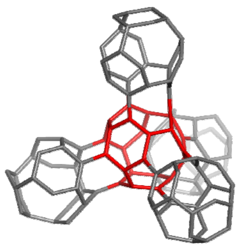
Design of structures was done by our original Nano Studio software (Nagy and Diudea, 2009).



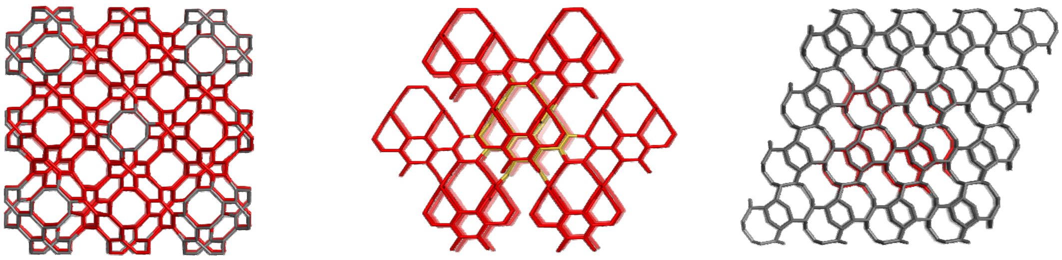
BTA.48



5BTA.196 Dendrimer



5BTZ.120 Dendrimer



BTA$_{fcc}$.333.864.Sel.17BTA

17BTA.624 Dendrimer

BTZ.444.1416.Sel.Ada.168

Figure. Polybenzenes as nano-dendrimers in early stages of crystal networks.

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References:

1. Diudea MV (2010) Nanomolecules and Nanostructures- Polynomials and Indices, MCM 10, Kragujevac.
2. Diudea MV, Katona G (1999), in: Newkome GA, Ed., Advan Dendritic Macromol 4:135-201.
3. Diudea MV, Nagy CL (2007) Periodic Nanostructures, Springer, Dordrecht.
4. Diudea MV, Petitjean M (2008) Symmetry in multi tori. *Symmetry Culture Sci* 19(4):285-305.
5. Nagy CL, Diudea MV (2017) Ring signature index. MATCH Commun Math Comput Chem *77* (2):479-492
6. Nagy CL, Diudea MV (2009) Nano Studio software program, „Babes-Bolyay“ University, Cluj.
7. O'Keeffe M, Adams GB, Sankey OF (1992) Predicted new low energy forms of carbon. Phys Rev Lett 68: 2325-2328.
8. Szefler B, Diudea MV (2012) Polybenzene multitori. Central Eur J Chem 10:1779-1785
9. Szefler B, Ponta O, Diudea MV (2012) Energetics of polybenzene multi tori. J Molec Struct 1022:89-93

REACTIVITY AND AROMATICITY OF POLYCYCLIC AROMATIC HYDROCARBONS' ISOMERS

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The chemical topology is connected with the chemical reactivity using the coloring method of matrix of atoms' adjacencies in molecules by standard reactivity indices i.e. electronegativity and chemical hardness, along with chemical power and the electrophilicity, which are used to describe bonding in a mechanistic/causal manner based on the first principles of quantum chemistry. The new proposed topo-reactivity coloring methodology further uses the fragments of atoms in molecules (the so called specific-bond-in-adjacency, SBA), single and double Carbon-Carbon bonds and in hetero-bounding Carbon and Hydrogen [1]. As application, a series of 16 polycyclic aromatic hydrocarbons (PAHs) and their isomers is analyzed from the present topo-reactivity methodology to yield the conclusion that the chemical power is the actual driving force triggering their reactivity, thereby refining previous molecular-orbital electronegativity-based approaches. On the other hand, in PAHs molecules, the aromaticity concept may be linked with their isomers conformation. In order to prove this theory, 16 PAHs molecules and their isomers were analyzed using the topo-reactivity method of specific-bond-by-adjacency procedure combined with Kekule, Clar, and Fries benzenoid descriptions. This way, a new method of classification for aromatic molecules was developed, which can be further applied in predicting which molecules are most likely to adopt the most aromatic conformation (of the Kekule-Clar-Fries type) in chemical reactions [2]. In this context, topo-reactivity methods are good candidates for research and developments in organic chemistry and chemistry of materials, in the XXIth-century quantum nanochemistry.

Keywords: *polycyclic aromatic hydrocarbons, topo-reactivity indices, aromaticity, isomers*

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REFERENCES

1. M. A. Tudoran, M. V. Putz, *Current Organic Chemistry*, **2015**, *19*, 359.
2. M. V. Putz, M. A. Tudoran, *Fullerenes, Nanotubes and Carbon Nanostructures*, **2016**, *24*, 733.

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Formation of Few-Layer Graphene by Pulsed Laser Ablation with Second Harmonic of Nd: Yag Laser in Liquid Nitrogen Medium

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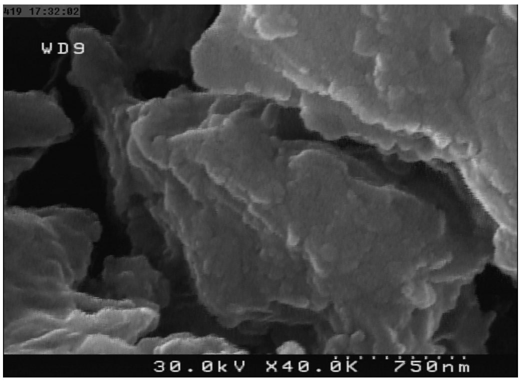
Graphene, a two-dimensional (2D) honeycomb lattice of carbon has attracted tremendous scientific interest in recent years due to their extraordinary electrical, mechanical, thermal and optical properties. In the present work, few-layer graphene nanosheets produced successfully by a simple and fast technique based on the pulsed laser ablation of graphite target in liquid medium using the Q-switched Nd:YAG laser at the wavelength of 532 nm and laser fluence of 1.8 J/cm^2. Structure and properties of the few-layer graphene nanosheets was studied using their UV–Vis–NIR absorption spectroscopy, Fourier transform infrared spectroscopy (FTIR), Field emission scanning electron microscopy (FESEM), Raman spectrum and transmission electron microscopy (TEM). The Raman spectroscopy indicates the formation of few-layer graphene nanosheets with graphitic domain size of 61.61 nm.

Keywords: *Graphene, Pulsed laser ablation, liquid nitrogen*, *TEM*

Figure. FESEM micrograph of the few-layer graphene nanosheets



REFERENCES

1. S. Bhandari, M. Deepa, A.G. Joshi, A.P. Saxena, A.K Srivastava, Nanoscale Research Letters, **2011**, 6, 424.
2. F. Tuinstra, J.L. Koenig ,Chem. Phys. **1970**, 53, 1126.