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Nano-Modeling of Strategic Materials for Knowledge Economy (NANO-MOD) - 2nd Edition

22 –23 April 2019, Timişoara

TABLE OF CONTENTS

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Nano-Modeling of Strategic Materials for Knowledge Economy (NANO-MOD) – 2nd Edition

22 –23 April 2019, Timişoara

Editor:

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NANO-MODELING OF STRATEGIC MATERIALS FOR KNOWLEDGE ECONOMY (NANO-MOD)

Timişoara (2019) 22-23 April

Research International Workshop
Second Edition

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PROGRAM & BOOK OF ABSTRACTS

2ND NANO-MODELING OF STRATEGIC MATERIALS FOR KNOWLEDGE ECONOMY: NANO-MOD

NANO-MOD *is a scientific and open forum in* nano-modeling of strategic materials for Knowledge (Frontier) Economy. Its objectives are in presenting the top-to date and the promotion on fundamental research and their societal implication from the MULTIDISCIPLINAR NANO-CHEMISTRY and TECHNOLOGY level (*non-limitative including the disciplines of physical-chemistry, chemical informatics, mathematical-chemistry, physical organic chemistry, nano-inorganic chemistry, biology-chemistry, biochemistry, bio-informatics, pharmaceutical chemistry, medical chemistry, ecotoxicology, geochemistry, QSAR, etc.*) – along they featured applications and products distributed, marketed and driving the Business Chemistry and related post-modern industries (i.e. *Nanotechnology:* Engineered Atoms, Super-Materials*; Biotechnology:* Technologically Created and Enhanced Life-Forms and Systems*; and 3D Printing:* Digitally Designed, Chemically Manufactured Objects), among others.

NANO-MOD (2nd Edition) 2019

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NANO-MOD 2019: PROGRAM

		Oral Presentations (P02Hall@FEAA**):**	
22 April 2019	9.30-10	**Mihai V. Putz** (*West University of Timişoara*)	*Opening*
(*Chairman*: Prof. Dr. M.V. PUTZ)	10.0-11.00	**Pablo D. Esquinazi** (*Felix-Bloch-Institute for Solid State Physics, University of Leipzig, Leipzig, Germany*)	*Interfaces in Graphite: A Roadmap towards room temperature Superconductivity*
	11-11.30	**Valentin Paul Nicu** (*"Lucian Blaga" University of Sibiu, Romania*)	*Implementation, Calculation and interpretation of Vibrational Circular Dichroism Spectra*
	11.30-12.00	**Ottorino Ori, Mihai V. Putz** (*Actinium Chemical Research Institute, Rome, Italy/ INCEMC - Timisoara, Romania/West University of Timisoara*)	*Topological Similarities Tori and Klein Bottle Nanostructures*
	12AM-12.30PM	**Break for Brunch (Lounge@FEAA)**	
		Oral Presentations (P02Hall@FEAA**):**	
22 April 2019	12.30-13.00	**Marilena Ferbinteanu and Fanica Cimpoesu** (*University of Bucharest/Institute of Physical Chemistry, Bucharest, Romania*)	*Electronic Structure Particularities of Lanthanide Ions in Molecules*
(*Chairman*: Dr. O. ORI)	13.00-13.30	**Cristina Tulbure** (*Banat University of Agriculture Sciences and Veterinary Medicine „King Michael I of Romania" Timişoara, Romania*)	*Education – A Frame Of Reference For The Knowledge Society*
	13.30-14.00	**Mihai V. Putz** (*West University of Timisoara/ INCEMC-Timisoara*)	*Orbital Clustering Method for Knowledge Management of Innovations*
22 April 2019	15.30-18.30	**Guest Research Workshop Dinner (*departure & location to be announced to the guest participants*)**	
		Oral Presentations (P02Hall@FEAA**):**	
23 April 2019	10-10.30	**M. Tolea, et al.** (*National Institute of Materials Physics, Bucharest-Magurele, Romania*)	*Hund rule or minimal spin in circular molecules and bipartite lattices*
(*Chairman*: CS1 Dr. F.Cimpoesu)	10.30-11	**Ana-Maria Putz et al.** (*"Coriolan Drăgulescu" Timisoara Institute of Chemistry, Romania*)	*Organically functionalised mesoporous silica for Hydrogen storage application*
	11-11.30	**Daniel Duda-Seiman et al.** (*University of Medicine and Pharmacy "Victor Babes" Timisoara*)	*Cost-effectiveness in the Era of Nano-Science in Biology, Medicine, and Pharmacy*
	11.30-12	**Adriana Isvoran et al.** (*West University of Timişoara, Romania*)	*Predictions Of The Molecular Targets And Side Effects Of The Degradation Products Of Chitosan*

23 April 2019	12AM-14PM	**Break for Brunch (Lounge@FEAA)**
	ORAL E-Posters' Presentations (P02Hall@FEAA**):**	
23 April 2019 (12AM-14PM, **Average 5 Minutes/ Poster Presentation)** **(*Chairman*: Dr. C. DUDA-SEIMAN)**	**P. D. Esquinazi et al.** (*Felix-Bloch-Institute for Solid State Physics, University of Leipzig, Germany*)	*Spin-filter device based on defect-induced magnetic homojunctions in ZnO*
	Cristina Maria Buta et al. (*Institute of Physical Chemistry, Bucharest, Romania*)	*The Modeling of Square-Pyramidal Mixed Ligand Copper Complexes*
	Ana M. Toader et al. (*Institute of Physical Chemistry, Bucharest, Romania*)	*Modeling of Cyanide-bridged Lanthanide-based Coordination Polimers*
	Adina Matica and Vasile Ostafe (*West University of Timisoara, Romania*)	*Antibacterial Effect of chitosan on Gram-positive and Gram-negative bacteria*
	Bianca-Vanesa Boros et al. (*West University of Timisoara, Romania*)	*Ecotoxicity Of Chitosan Nanoparticles On Lemna Minor And Daphnia Magna*
	Gheorghita Menghiu and Vasile Ostafe (*West University of Timisoara, Romania*)	*Chitinases: An Option For The Future Of NanoMedicine, NanoBiotechnology And NanoAgriculture*
	Liana Stefan and Corina Duda-Seiman (*West University of Timisoara, Romania*)	*Medical translation between accuracy and imposture*
	Nicoleta Săculțeanu et al. (*West University of Timisoara, Romania*)	*Preliminary Studies On Chitosan Based Membrane Composites*
	Marin Roman et al. (*West University of Timisoara, Romania*)	*Prediction Of The Pharmacological Profiles Of Some Oligomers Of Lactic Acid. A Computational Study*
	Paula Svera et al. (*INCEMC - Timisoara, Romania/ University Politehnica of Timişoara*)	*The Influence Of Organic Stabilizators In The Water Splitting Process Using Semiconductor Photocatalysts*
	Mihai V. Putz et al. (*West University of Timisoara, Romania/INCEMC-Timisoara*)	*Optimizing device of logical matrices towards semiconductivity*
	Mihai V. Putz et al. (*West University of Timisoara, Romania/INCEMC-Timisoara*)	*Chemical Reactivity Driving Switchable Molecular Machines*
	Marina A. Tudoran and Mihai V. Putz (*West University of Timisoara, Romania/INCEMC-Timisoara*)	*Green's Function In Modeling Graphenic Chemical Bonds*
	Diana Larisa Roman et al. (*West University of Timisoara, Romania*)	*Assessment Of The Human Hazard Of Some Oligomers Of Polyhydroxyalkanoates*
	Alina-Maria Petrescu et al. (*West University of Timisoara, Romania/OncoGen Centre, County Hospital "Pius Branzeu", Timisoara, Romania*)	*LD/MM+ Simulation Of Some Coupled Species In Box Water*

NANO-MOD 2019:

ABSTRACTS

~ ORAL PRESENTATIONS ~

Abstract/Graphical Abstract

INTERFACES IN GRAPHITE: A ROADMAP TOWARDS ROOM TEMPERATURE SUPERCONDUCTIVITY

Pablo D. Esquinazi
Felix-Bloch-Institute for Solid State Physics, University of Leipzig, Leipzig, Germany

ABSTRACT

Usual graphite samples, independently whether they are from natural sources, Kish or highly oriented pyrolytic graphite, bulk or powder samples, have interfaces. These interfaces occur between twisted regions with Bernal or rhombohedral or between Bernal and rhombohedral stacking orders. I discuss (very) old and new results - from single interfaces (bilayer graphene[1]) to multigraphene and bulk or powder graphite samples[2] - that speak for the existence of superconductivity with a broad distribution of critical temperatures. Especial emphasis will be given to new results, which indicate the existence of granular superconductivity even above room temperature[3-4].

Keywords: graphite, interfaces, superconductivity

ABSTRACT FIGURE

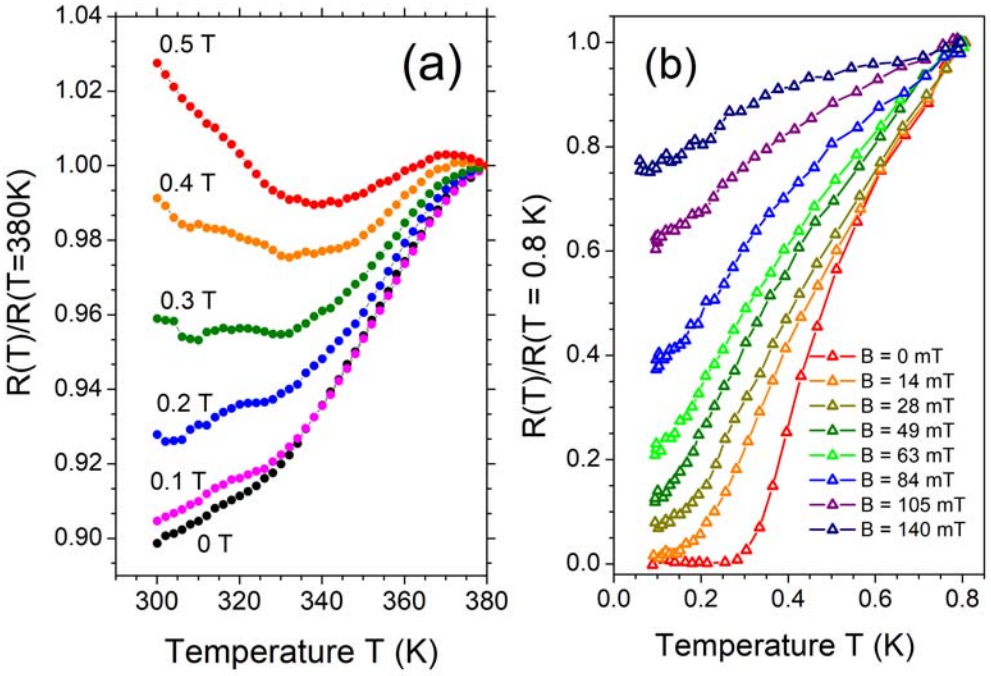

Figure: Normalized resistance vs. temperature at constant magnetic fields applied normal to the graphene planes and interfaces of the following samples: (a) natural graphite sample; data taken from Fig. 6(b) in [3]. (b) Bilayer graphene device M2 (twist angle θ = 1.05°), data taken from Fig. 1(b) in [1].

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Abstract/Graphical Abstract

IMPLEMENTATION, CALCULATION AND INTERPRETATION OF VIBRATIONAL CIRCULAR DICHROISM SPECTRA

Valentin Paul Nicu
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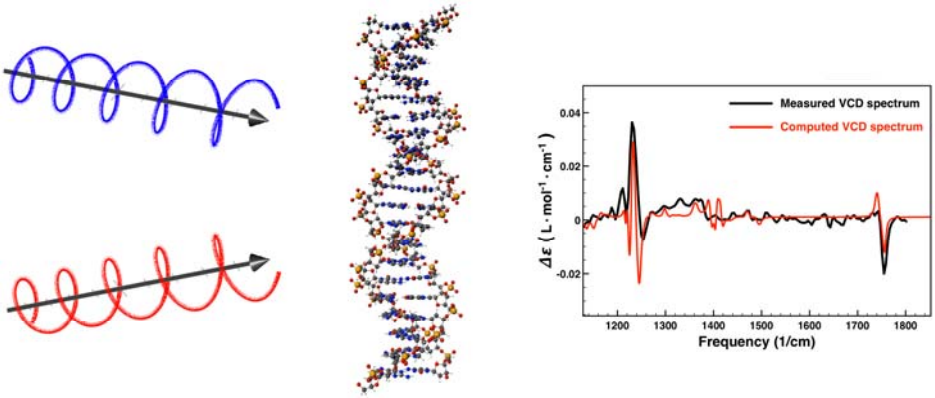
ABSTRACT

Vibrational Circular Dichroism (VCD) spectroscopy, the difference between the absorption of left and right circularly polarized light during a fundamental vibrational transition, is able to differentiate the non-identical mirror images of a chiral molecule. First, the details of the implementation of the VCD equations into the Amsterdam Density Functional program package will be presented. Then, the usefulness of this implementation will be demonstrated by considering a broad range of molecules, i.e., from flexible organic molecules to inorganic compounds and to gold clusters. The good agreement obtained between the experimental and simulated VCD spectra of the considered example molecules, demonstrated clearly that VCD is a reliable spectroscopic technique that allows one to differentiate the enantiomers (i.e., non-identical mirror images) of chiral compounds.

Keywords: Vibrational Circular Dichroism, Chirality, DFT



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*NEW FRONT CHEM 28 (**2019**) 1-66*

2nd Nano-Modeling of Strategic Materials for Knowledge Economy
Book of Abstracts

Abstract/Graphical Abstract

TOPOLOGICAL SIMILARITIES TORI AND KLEIN BOTTLE NANOSTRUCTURES

Ottorino Ori **[1,2]** **, *Mihai V. PUTZ*** **[1,3,♣]**

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[2] Laboratory of Renewable Energies – Photovoltaics, INCEMC - National Institute for Research and Development in Electrochemistry and Condensed Matter, Dr. A. Păunescu Podeanu Street No.144, 300569 Timisoara, Romania
[3] Laboratory of Structural and Computational Physical-Chemistry for Nanosciences and QSAR, Biology-Chemistry Department, West University of Timisoara, Pestalozzi Street No. 16, Timisoara, RO-300115

ABSTRACT

Distance based topological invariants like the Wiener number and the topological roundness have been computed for hexagon-tiled tori and Klein bottles (also called toroidal and Klein bottle fullerenes) that are described therefore as closed graphs with N vertices and $3N/2$ edges in which N depends on the variable length of the cylindrical edge L_C of these nanostructures where the length L_M of the Möbius zig-zag edge is kept constant. Current results show that this family of Klein bottle cubic graphs, over a certain threshold size ~~L_C~~ get assimilated to the toroidal lattices with the same size (N, L_C, L_M) in the sense that both nanostructures share the *same* values of the topological indices that measure graph compactness and roundness, two key topological properties largely influencing lattice stability. Moreover, this newly reported topological similarity between the two kinds of graphs, transfers the *translation invariance* typical of the graphenic tori to the Klein bottle polyhexes with size $L_C \geq$ ~~L_C~~ making these graphs *vertex transitive*. This means that a traveler jumping on the nodes of these Klein bottle fullerenes is not able any more to distinguish among them just measuring the chemical distances. This size-induced *symmetry transition* for Klein bottle cubic graphs represents a relevant topological effect influencing the electronic properties and the theoretical chemical stability of these two families of graphenic nanosystems. Some preliminary conclusions on this matter are also drawn.

Keywords: Topological Invariants, Tori fullerenes, Klein Bottle fullerenes.

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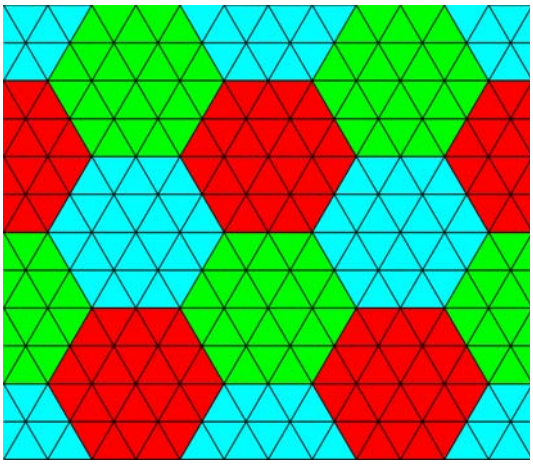
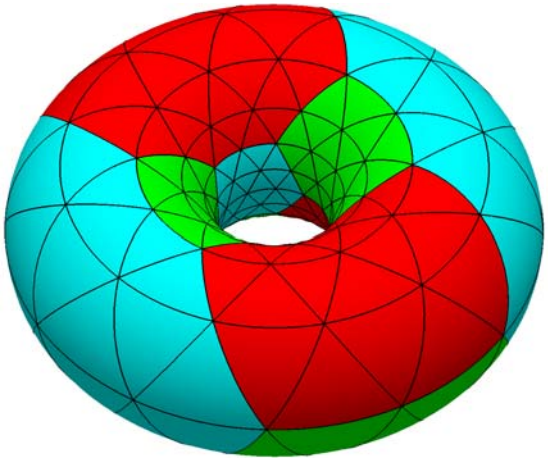
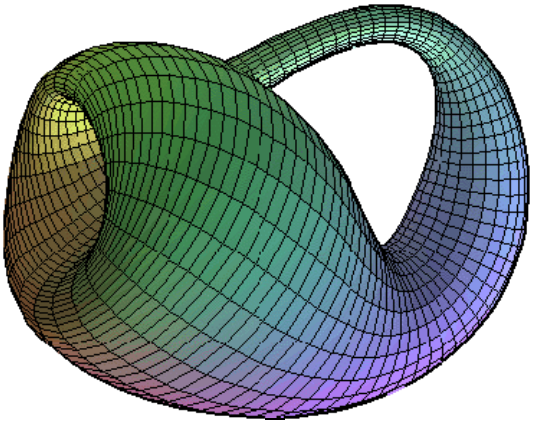
ABSTRACT FIGURE







ACKNOWLEDGEMENT

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Abstract/Graphical Abstract

ELECTRONIC STRUCTURE PARTICULARITIES OF LANTHANIDE IONS IN MOLECULES

***Marilena Ferbinteanu*[1*], *Fanica Cimpoesu*[2*]**
[1] Faculty of Chemistry, Inorganic Chemistry Department, University of Bucharest, Dumbrava Rosie 23, Bucharest 020462, Romania.
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ABSTRACT

The lanthanides are key elements in several modern and future targeted applications, based on their magnetic and optical properties. The rational structure-property correlations represent an elegant way to engineer desired functionalities, starting from first-principle fundaments. However, hidden drawbacks are staying in the way to such desiderata, springing from the peculiarities of f-shell of lanthanide ions: non-*aufbau* configuration and weak interaction with the environment, demanding non-routine approach by electron structure methods. We claim pioneering breakthroughs in this field, [1, 2] continued with many relevant case studies based on the synthetic outcome of the first author and methodological advances of the second one.

Keywords: Lanthanide Complexes, Ligand Field, Ab Initio, Magnetism, Luminiscence

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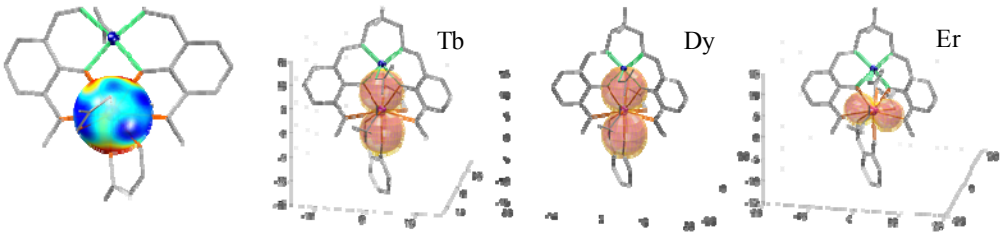

Fig. 1. Ligand Field and magnetization maps a series of Cu-Ln compexes (Ln=Tb, Dy, Er).

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Abstract/Graphical Abstract

EDUCATION – A FRAME OF REFERENCE FOR THE KNOWLEDGE SOCIETY

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ABSTRACT

Education represents a fundamentally individual and social value which is currently going through a process of multiple reconstruction. In an era where the only constant is the change, education is called to train individuals able to successfully integrate into the knowledge society. In this context, education on all its levels, mainly the higher level, is responsible for building some competencies and key-attitudes that will allow the graduate to continually adjust to the social and professional environment in which they are to integrate. As it is mentioned in the official statement at London (2007), the contemporary world found in its continual change prescribes the need to adjust the systems of higher education in order to efficiently answer the challenges of globalization. More precisely, according to Chivu (2008), the main finalities grounding the 3rd millennium's education are: the forming abilities to participate and anticipate, the critical and self-critical spirit; the introspection and acting according to values such as: tolerance, solidarity, cooperation, acceptance of cultural diversity; building and developing the capacity and availability for dialogue, the skill to establish the contact between cultures and groups. In his work entitled *21 Lessons for the 21st Century,* the History teacher Harari (2018) claims that the contemporary Pedagogy has to emphasize the 4 Cs: critical thinking, communication, collaboration, creativity. In order to achieve these aims, the process of training teachers has to be completely reformed, in a way in which the student-centered strategies have the precedence: active-participatory creative strategies, team-work strategies, strategies of accountability and communication at all levels and in all forms. Obviously, unitary instruction that used to dominate the traditional education needs to be replaced by differentiated instruction according to the following criteria: the students' level of training; the interest for certain domains; specific needs and learning styles. In this context, the universities will re-think their curriculum from the perspective of student-centered instruction, teaching-learning and assessment focused on competencies, by creating some differentiated and flexible curricular lines (Singer and Sarivan, 2006). On the whole, the 3rd millennium education will be focused on building cross

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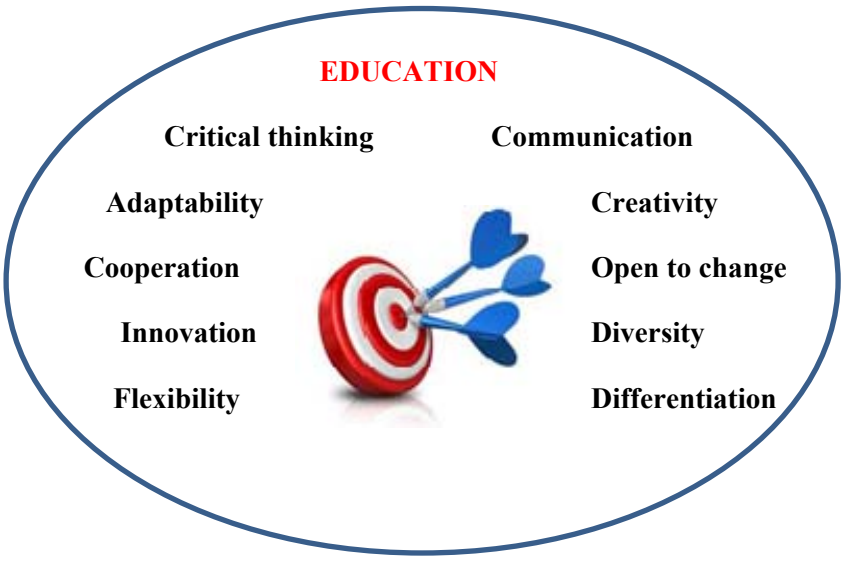
competencies such as adjustment to change, permanent learning and on maintaining the mental balance in an extremely dynamic world.

Keywords: education, knowledge society, student-centered instruction, key-competencies.

ABSTRACT FIGURE



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Abstract/Graphical Abstract

ORBITAL CLUSTERING METHOD FOR KNOWLEDGE MANAGEMENT OF INNOVATIONS

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ABSTRACT

The actual and future nano-, quantum-, and meta- postmodern eras (viz. William Gibson: „*The future is already here — it's just not very evenly distributed*”) identify of the trans-disciplinary methods, especially from maths, physics, biology and chemistry, driving and designing the realities and facing the actual-future (viz. an Amerindian quote: „*to a new music a new dance is needed*!”) in a open-closed space: open, due to the open-access in a network, but close since conditioned by the knowledge to the network (code, cipher). Accordingly, a “heroic” conception of the many-fold Strategy of the truth (the so called Knowledge Management), usually associated with teleological truth (i.e. “the truth is out there”) and with the revolutions in scientific development, as proliferated by Popper and then by Kuhn, is currently re-cognized as merely a (continuous) RE/DE/RETROevolution, made by trial and error with the aid of “little management” contribution(s) around big or fundamental conceptions of Nature, so defining the *Strategic Clustering of Knowledge*. It aims to clarify the post-modern approach of science in general and of knowledge economy in special; in this post-modern context, the periphery is becoming center, i.e. the new “escaping center”, re-accelerating (by gravitation) the central knowledge concepts of a circle (taken for instance as the nano-tech, nano-chemistry, or nano-economy) in developing eccentricity on ellipses and with key innovation and critically equilibrating the attraction to center or to periphery on a hyper-bolas of a scientific “planetarium system”; such a framework may constitute a basis for a dynamic potential theory in nano-technological (meta)clustering of XXI century within the actual “8th orbits on a planetarium model” as the general clustering of knowledge management. It may eventually trigger new algorithm by which nano-innovations (involving

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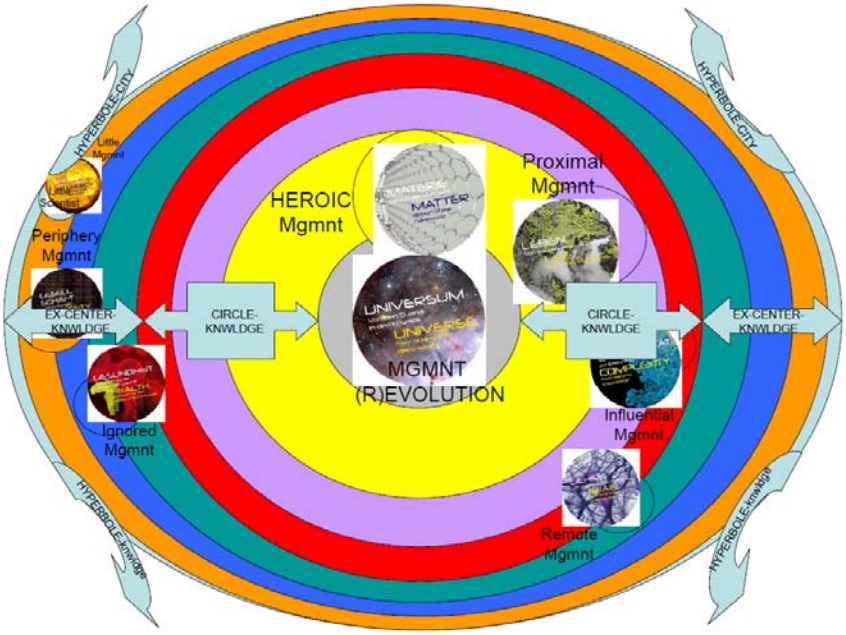
both science and management of science) may be strategically structured and emerged by the planetarium clustering method.

Keywords: Strategic management, Intelligent coopetition, GLocal effects, Orbital System

ABSTRACT FIGURE



ACKNOWLEDGEMENT

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Abstract/Graphical Abstract

HUND RULE OR MINIMAL SPIN IN CIRCULAR MOLECULES AND BIPARTITE LATTICES

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ABSTRACT

Hund rule's relevance has long exceeded the boundaries of atomic physics where it was first formulated, over the years being investigated in many other systems such as quantum dots [1], artificial molecules created by quantum dots [2], metal clusters [3], bipartite lattices [4, 5], trilayer graphene [6], etc.

In this paper we discuss the spin properties of circular molecules with an arbitrary number of atoms whose one-particle spectrum, in general, shows a ladder of double degenerate electronic states. We show [5] that an anti-Hund rule always defines the ground state in a circular molecule with 4N atoms at half-filling. In all other cases (i.e. number of atoms not multiple of four, or a 4N molecule away from half-filling) both the singlet and the triplet outcomes are possible, as determined primarily by the total number of electrons in the system. In some instances, the Hund rule is always obeyed and the triplet ground state is realized mathematically for any values of the on-site and long range interactions, while for other filling situations the singlet is also possible but only if the long-range interactions exceed a certain threshold, relatively to the on-site interaction.

In a celebrated paper, E. Lieb [7] gives exact results regarding the net spin of a so-called bipartite latice (i.e. which can be divided in "A" and "B" sub-groups of sites, hopping existing only between sites from different sub-groups) at half filling, in the presence of on-site Hubbard interaction. We study [8] the validity of the Lieb rule for a generalized Hamiltonian (including long-range interactions) using perturbatives plus Configuration-Interaction approaches.

Keywords: Hund Rule, Circular Molecules, Configuration-Interaction, Lieb lattices

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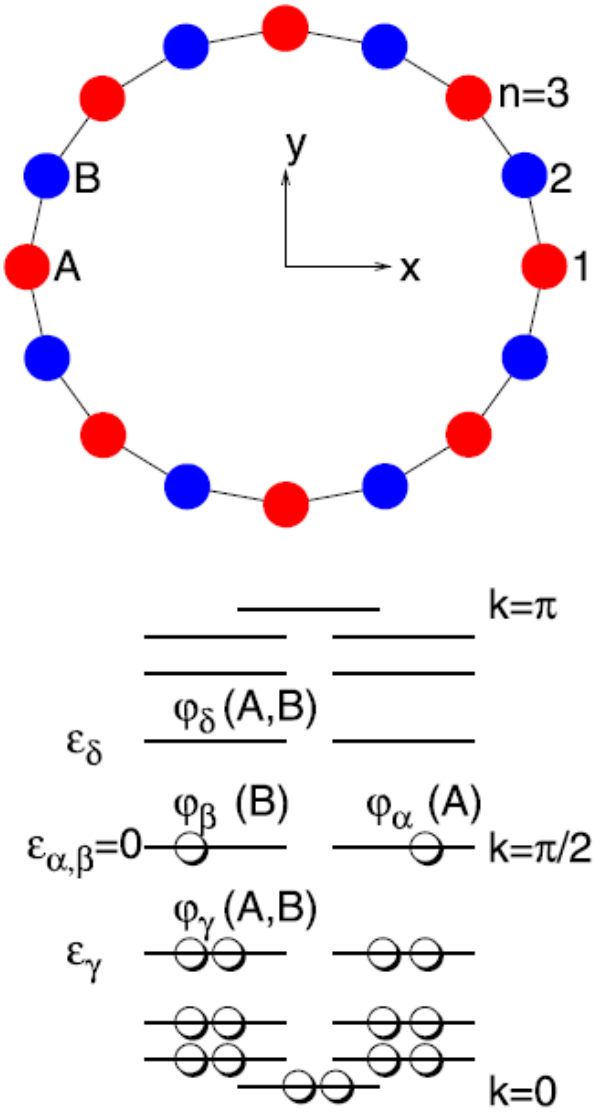

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Abstract/Graphical Abstract

ORGANICALLY FUNCTIONALISED MESOPOROUS SILICA FOR HYDROGEN STORAGE APPLICATION

Ana-Maria Putz [♣1] ***Alfonso Policicchio*** [2,3,4†], ***Raffaele G. Agostino*** [2,3,4], ***Sara Stelitano*** [2], ***Giuseppe Conte*** [2], ***Cătălin Ianăşi*** [1], ***Bogdan Ţăranu*** [5], ***Marius Mirică*** [5]

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ABSTRACT

The H_2 adsorption properties of prepared functionalized porous silica with different compositions have been studied. Mesoporous silica particles were synthesized by using the sol-gel method, with tetradecyltrimethyl ammonium bromide (C14) or dodecyl trimethyl ammonium bromide (C12) as structure directing agents from tetraethoxysilane (TEOS) and methyltriethoxysilane (MTES) precursors, by varying the molar ratio of the silica precursors. The porosity and microstructure of the materials in function of the MTES/TEOS ratio were evaluated by using nitrogen adsorption, and the transmission electron microscopy method. The textural characterization was performed in order to connect their properties to possible applications as hydrogen adsorptive materials.

The ability of a material to store gas molecular species may not only be governed by on the specific surface area but also by the porosity and to the possibility to form more than one monolayer of adsorbed gas molecules. These are the reasons why the evaluation of the adsorbed hydrogen molecules per nm^2 could be useful to indicate the efficacy of the samples to create more than one monolayer [1].

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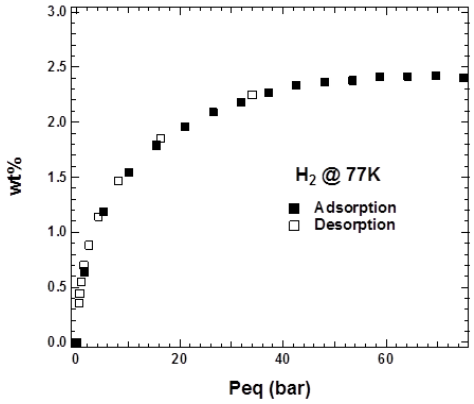
Improving the interaction between adsorbent and adsorbate is the breakthrough for synthesizing an optimum hydrogen storage material [2]. Thus, studies on physisorption materials aim to increase surface area, optimize the pore diameter, and increase the affinity toward incoming hydrogen molecules through the introduction of atoms and/or molecular groups into the porous material. A previous study had been demonstrated that the amorphous structure of the adsorbent and the use of shorter surfactant molecules in the synthesis increased both the storage capacity and the strength of the interaction between the surface and the adsorbate [1]. In our previous study the data analysis shows that the methyl functionalized sample, according to its structural parameters is the best material either from the point of view of maximum adsorption capacity showed for H_2 [3]. The higher adsorption capacity of the samples synthesized with no MTES and with C12 directing agent can be debited to a different and stronger sorbent-adsorbent interaction beyond that slightly differences in the textural properties.

In the C14 directing agent series of samples, the sample with no MTES and the samples with low amount of MTES, appears the most performing at 77K immediately followed by the samples synthesized with increase amount of MTES. In each series of samples, C12 and respectively C14, the samples show different grade of interaction with the incoming H_2 molecules (*K*) and different values of homogeneity (*t*). The distance between two pore centers of parallel pore channels was estimated from TEM at: 3.3 nm for all samples from C12 series. Therefore, the inter-pore distanced is almost the same with the addition of small amounts of MTES, in the present synthesis conditions.

Keywords: hydrogen storage, functionalized mesoporous silica, transmission electron microscopy.



Abstract Figure. *Adsorption-desorption isotherm obtained on one of the samples (synthesized with low amount of MTES) at T = 77K up to 80 bar. Close box = adsorption, open box = desorption.*

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Abstract/Graphical Abstract

COST-EFFECTIVENESS IN THE ERA OF NANO-SCIENCE IN BIOLOGY, MEDICINE, AND PHARMACY

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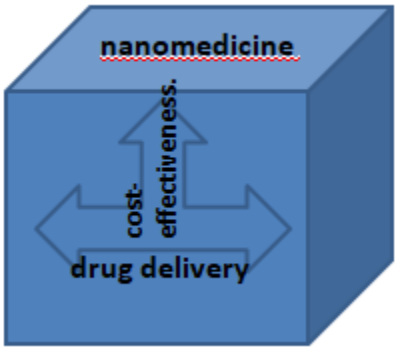
ABSTRACT

To implement a new bioactive compound as a pharmaceutical agent (drug), it requires a prolonged process, starting from computer assisted drug design, synthesis, preclinical and clinical trials, post-marketing studies. Each phase implies impressive logistics, both human and technical, with significant costs. A correct economical profile compares the costs of these phases, the outcomes of the analyzed drug with a relevant already marketed same- or related-class medicine.



Generic drugs are a real cost-effective option if they meet the criteria of bioequivalence.
Nanoparticles have an unique feature, namely to improve the diagnostic course and the treatment in a given disease. The Joint Research Center of the European Comission evaluated that more than 50% of new patents refer to the segment of drug delivery. Sales for all nanomedical products were estimated at US$110 billion in 2016. [1]
In cancer research, challenges are very high. There is still a very low probability for success (6%) that a small molecule passes all the way from pre-clinical proof to commercial launch when anti-cancer drugs are discussed. [2]. It is a long way to go in order to obtain potent drugs, and this is feasible applying new nano-techniques in biology, medicine, and pharmacy.

Keywords: nanomedicine, drug delivery, cost-effectiveness.

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NANO-MOD **2019**
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2nd Nano-Modeling of Strategic Materials for Knowledge Economy
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Abstract/Graphical Abstract

PREDICTIONS OF THE MOLECULAR TARGETS AND SIDE EFFECTS OF THE DEGRADATION PRODUCTS OF CHITOSAN ‡

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ABSTRACT

Chitin is a polysaccharide abundantly found in nature, especially in seafoods, but also in insects and fungi. Chitosan is obtained from chitin by chemical or enzymatic deacetylation. The difference between chitin and chitosan consists of the acetyl content, chitin contains mostly N-acetyl-D-glucosamine units and chitosan contains especially D-glucosamine. Chitin and chitosan reveal biocompatibility, biodegradability, and non-toxicity for humans and environment, their anti-fungal, anti-bacterial, anti-microbial and anti-oxidant properties conducting to numerous medical applications [1]. Chitosan polymers introduced into the body through food or drugs are degraded to oligomers that are released into the human body. These chitosan oligomers (COs) vary in the degree of polymerization (DP), the degree of deacetylation (DAC) and the deacetylation pattern (DAP) [2]. We have predicted the molecular targets of chito-oligomers containing up to 8 monomeric units using Swiss Target Prediction [3] and their side effects using Prediction of Activity Spectra of Substances [4] computational tools. The overview of the molecular targets of investigated COs reveals that they belong to the following classes: enzymes, adhesion proteins, secreted proteins, cytosolic proteins, membrane receptors, kinases, and unclassified proteins. There are some dissimilarities between the identified molecular targets for chito-oligosaccharides with distinct MW, DAC, and DAP. As the molecular weight increases, the more diverse is the spectrum of the identified molecular targets. Predicted side effects of investigated COs are weight loss, gastrointestinal and respiratory disorders, reproductive dysfunctions, necrosis, and neurotoxicity.

Keywords: chitin, chitosan, molecular targets, side effects

‡ This work was supported by Grant: PNIII-P3-285 Polymeric NanoBioMaterials for drug delivery: developing and implementation of safe-by-design concept enabling safe healthcare solutions – GoNanoBioMat

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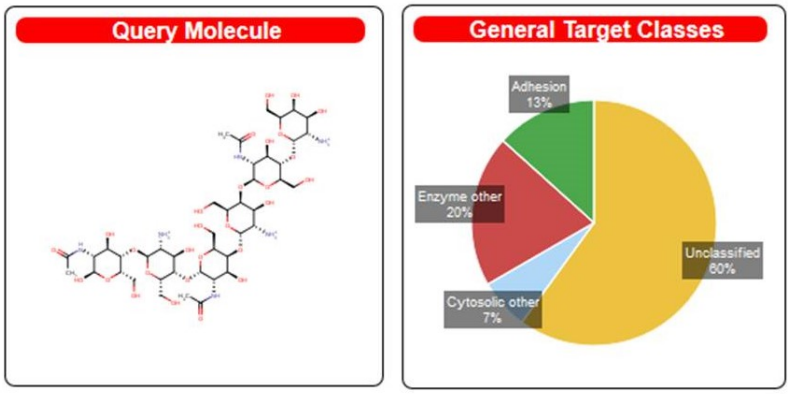
ABSTRACT FIGURE



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ABSTRACTS

~ ORAL POSTERS ~

Abstract/Graphical Abstract

SPIN-FILTER DEVICE BASED ON DEFECT-INDUCED MAGNETIC HOMOJUNCTIONS IN ZNO

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ABSTRACT

After more than a decade of extensive research on the magnetic order triggered by lattice defects in a wide range of nominally non-magnetic materials[1], we report its application in a spintronic device[2]. This device is based on a spin-filter phenomenon we have discovered at the interfaces between defect-induced magnetic regions, produced at the surface of a Li-doped ZnO microwire by low-energy proton implantation, and non-magnetic regions. Giant positive magnetoresistance larger than 500% is observed at 300~K and magnetic fields ~100Oe. The effect scales with the number of interfaces introduced along the wire and depends on the implantation dose. By modelling the transport through the magnetic/non-magnetic interfaces, the magnetic exchange coupling strength between localized magnetic defects is calculated and compared to coupling strengths of ferromagnetic materials found in the literature.

Keywords: defect-induced magnetism, ZnO, magnetoresistance

ABSTRACT FIGURE

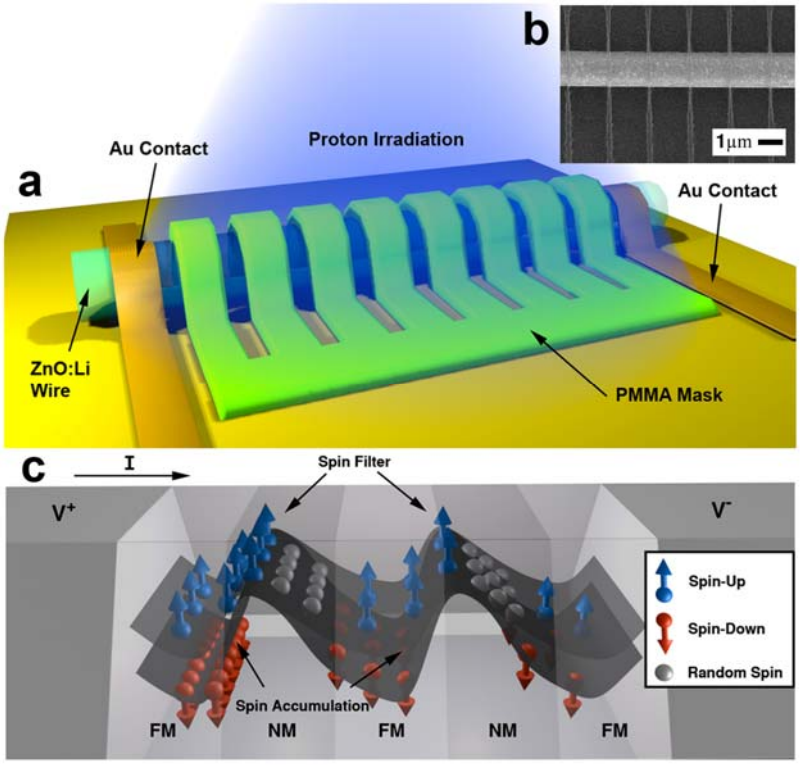

Figure: (a) Schematic of the H^+ implantation process to produce defect-induced magnetic strips on the surface of a ZnO:Li microwire. The PMMA mask is produced by electron beam lithography to achieve structure sizes down to 100nm. (b) SEM picture of a wire with a mask covering 100nm long regions for the creation of alternating magnetic/non-magnetic stripes by proton implantation. (c) Sketch of the phenomena that contribute to the large magnetoresistance: The potential wells between the magnetic (FM) and non-magnetic (NM) regions produce a spin accumulation and spin filtering at the boundaries. These lead to a sign change (relative to the FM path) and a large increase of the magnetoresistance along the wire main axis.

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Abstract/Graphical Abstract

THE MODELING OF SQUARE-PYRAMIDAL MIXED LIGAND COPPER COMPLEXES

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ABSTRACT

Two new mixed-ligand copper complexes with 1,10-phenanthroline and monodentate pyrazoles (3,5-dimethyl-4-*R*-pyrazole, where *R* = nitro or iodo), stand as case-studies for a revisited view on Ligand-Field (LF) qualitative and semi-quantitative issues [1], brought in conjunction with the rich information offered by the state-of-the art computational methods [2]. The combined analysis of the first TD-DFT energies and density difference maps (see an example in Fig.1a) enables a scheme of the LF split.

A suggestive representation of the anisotropic quasi-tetragonal gyromagnetic tensor is given in Fig. 1b. The experimental EPR spectrum and the computed parameters are shown in Fig. 1c. Clear correlations are drawn between computed and experimental UV-VIS and EPR spectra, rationalizing the Landé factors in terms of Ligand Field states.

Keywords: Cu(II) complexes, Ligand Field models, TD-DFT calculations, EPR spectra.

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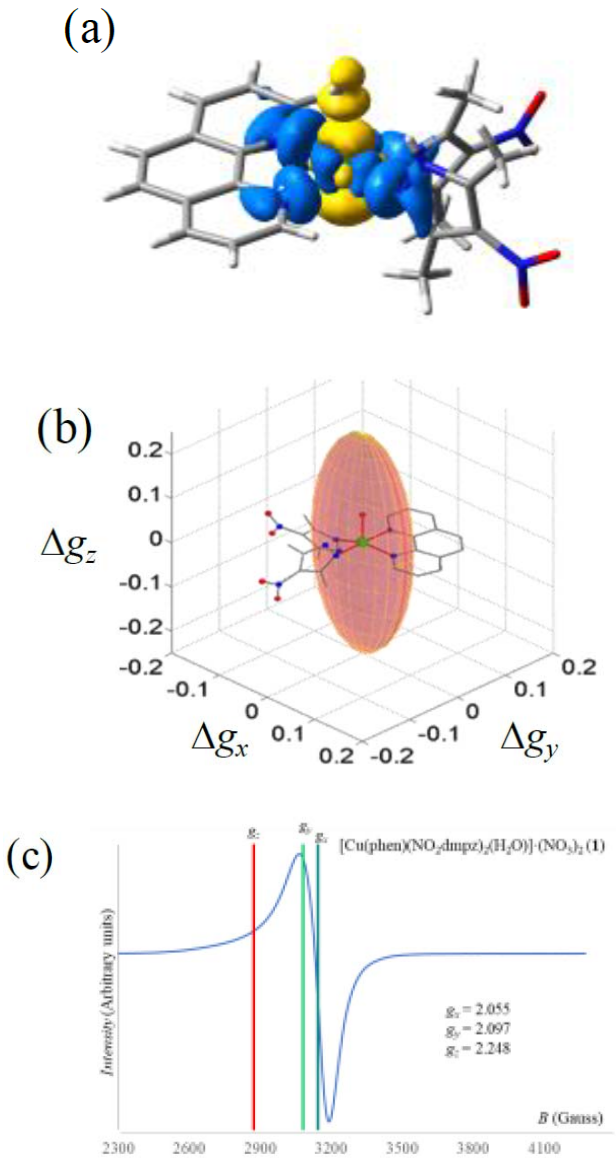

Fig. 1. Synopsis of performed measurements and calculations.

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Abstract/Graphical Abstract

MODELING OF CYANIDE-BRIDGED LANTHANIDE-BASED COORDINATION POLIMERS

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ABSTRACT

The cyanide-bridged molecular assemblies containing lanthanide ions are gaining increased interest due to their multifunctional properties, particularly those based on magnetic anisotropy. We present the theoretical analyses for a series of isostructural compounds based on pyrazine-2,3-dicarboxylic acid (2,3-H2pzdc) as linker, having the general formula: $\{KH[Ln_2(2,3\text{-}pzdc)_2(CH_3OH)(H_2O)_7][M(CN)_8]\}\bullet nH2O$ (Ln3+ = Nd, Gd, Tb, Dy; M4+ = Mo, W). [1]

Keywords: Lanthanide Complexes, Magnetic Anisotropy, Ligand Field.

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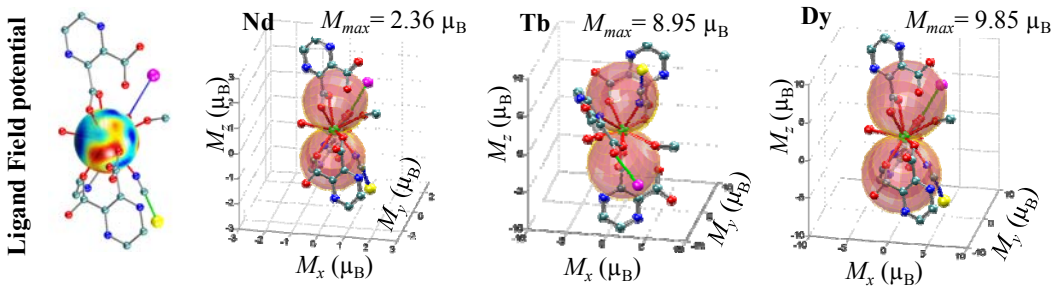

Fig. 1. Ligand Field and magnetization maps of site 1 in discussed systems.

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Abstract/Graphical Abstract

ANTIBACTERIAL EFFECT OF CHITOSAN ON GRAM-POSITIVE AND GRAM-NEGATIVE BACTERIA

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ABSTRACT

Chitosan is one of the most used biopolymers in biomedical applications due to its high biocompatibility, biodegradability and strong antimicrobial properties. Due to its cationic nature, chitosan can interact with negatively charged components of the bacterial cell surface. Although chitosans mechanism of action on bacteria is yet to be fully understood, the most prevalent proposed mode of action is based on electrostatic interactions between positively charged NH_3^+ groups of N-acetyl-D-glucosamine units from chitosan and highly negatively charged lipopolysaccharides present in the bacterial cell. Chitosan may alter the cell membrane permeability, leading to cell death, either by causing the leakage of cytoplasmic content or by entering the cell followed by attachment to the negatively charged nucleic acids and interfering with their roles in the cell. Recently, a great interest has been showed on developing nanoparticles based on chitosan as an alternative to conventional antibiotics, in order to fight microbial resistance. The aim of this study was to evaluate the antibacterial activity of chitosan solution and chitosan nanoparticles against Gram-positive bacteria (*Staphylococcus aureus*) and two strains of Gram-negative bacteria (*Escherichia coli* and *Pseudomonas aeruginosa*). Chitosan nanoparticles were prepared using ionic gelation method and the antibacterial effect was determined by measuring the Minimum Inhibitory Concentration (MIC) and Minimum Bactericidal Concentration (MBC). As expected, chitosan demonstrated antibacterial activity, both in solution and nanoparticle form, chitosan nanoparticles exhibiting higher inhibitory effect. All bacterial strains were inhibited by chitosan, Gram-positive bacteria being more sensitive than Gram-negative ones.

Keywords: chitosan, nanoparticles, ionic gelation, antibacterial

Acknowledgement: This work was supported by Grant: PNIII-P3-285 Polymeric NanoBioMaterials for drug delivery: developing and implementation of safe-by-design concept enabling safe healthcare solutions – GoNanoBioMat

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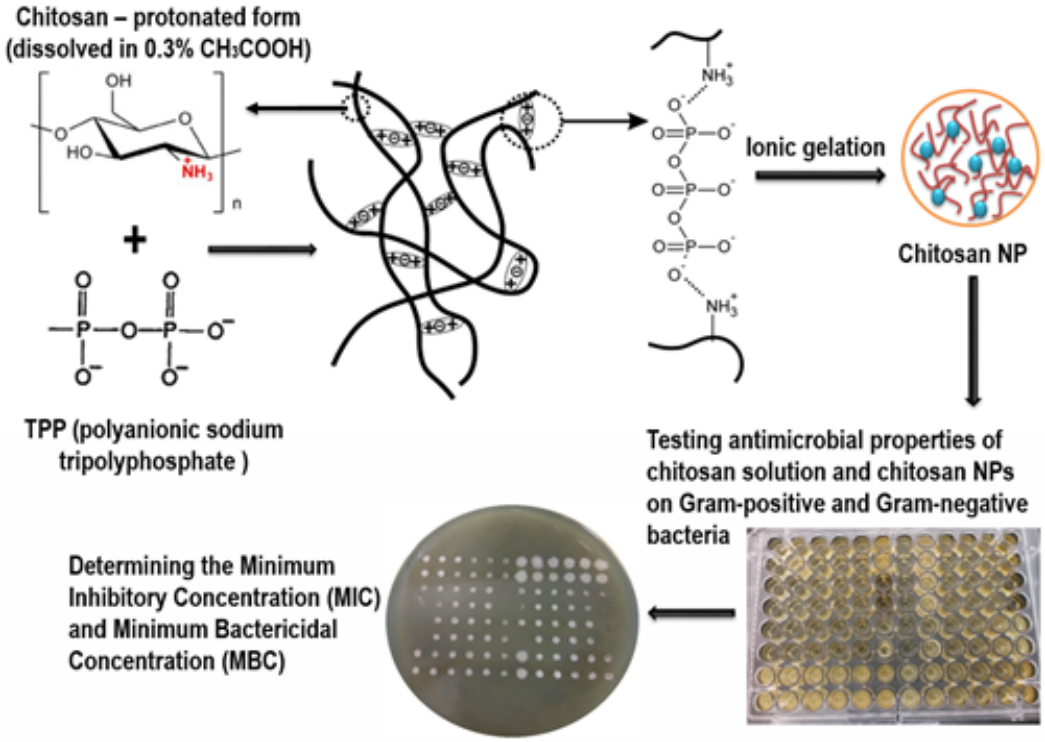

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2nd Nano-Modeling of Strategic Materials for Knowledge Economy
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Abstract/Graphical Abstract

ECOTOXICITY OF CHITOSAN NANOPARTICLES ON *LEMNA MINOR* AND *DAPHNIA MAGNA*

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[2] West University of Timisoara, Advanced Environmental Research Laboratories

ABSTRACT

The ecotoxicity of chitosan nanoparticles was assessed using a growth inhibition assay on *Lemna minor* and an acute toxicity assay on *Daphnia magna*. The tests also included acetic acid as a solvent control which was used in the manufacturing of the chitosan nanoparticles. The results of the *Lemna* assay enabled the plotting of a dose-response curve for both chitosan and acetic acid. The EC_{50} values showed that chitosan (0.03%) was slightly more toxic than acetic acid (0.036%), which shows a possible contribution of acetic acid to chitosan's toxicity. The results of the *Daphnia* assay enabled the plotting of a dose-response curve only for chitosan at 24-hour exposure, as 48 hours assay indicated that the mortality for chitosan was 100% for all concentrations. The results have shown that the most sensitive assay for both chitosan nanoparticles and acetic acid was the *Daphnia* assay at 48 hours. Both chitosan and acetic acid were the least toxic to duckweed. The highest toxicity of chitosan was observed for daphnids at 24 hours with EC_{50} value of 0.012%, chitosan being 2.5 times more toxic to daphnids than duckweed.
This work was supported by Grant: PNIII-P3-285 Polymeric NanoBioMaterials for drug delivery: developing and implementation of safe-by-design concept enabling safe healthcare solutions – GoNanoBioMat

Keywords: ecotoxicity assessment, *Daphnia* acute toxicity assay, *Lemna* growth inhibition assay, chitosan, chitosan nanoparticles

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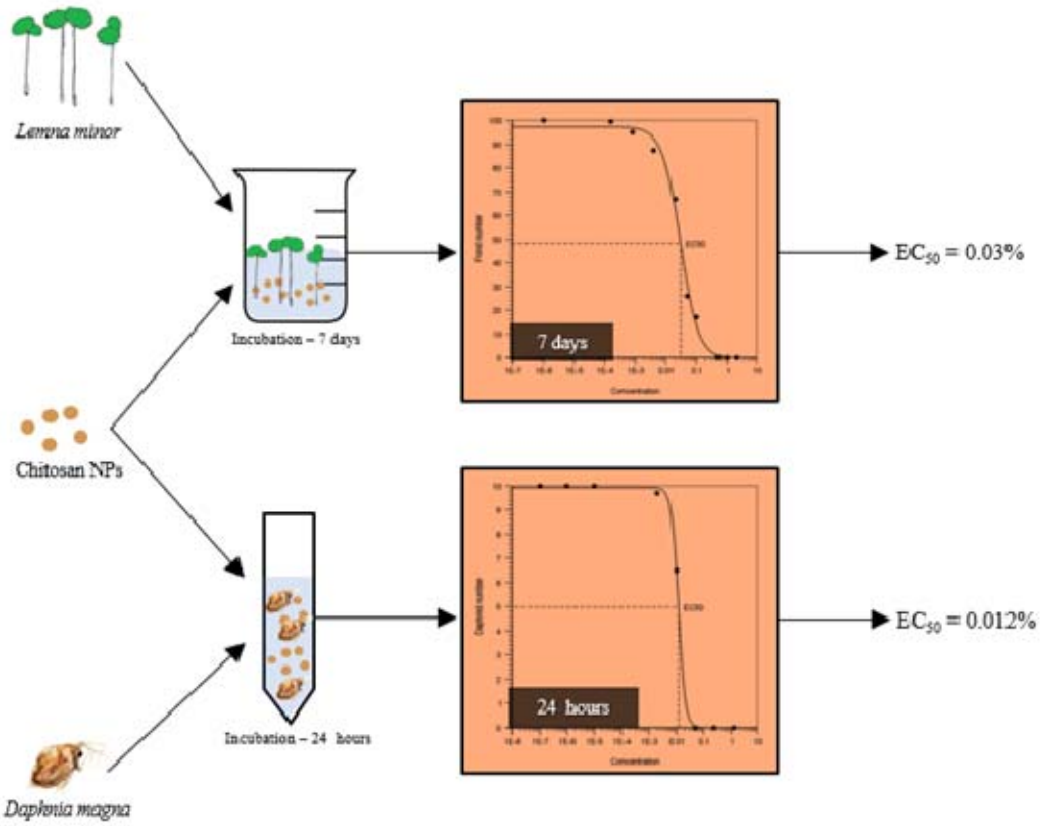
ABSTRACT FIGURE



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NANO-MOD **2019**
22-23 April, Timişoara
*NEW FRONT CHEM 28 (**2019**) 1-66*

Abstract/Graphical Abstract

CHITINASES: AN OPTION FOR THE FUTURE OF NANOMEDICINE, NANOBIOTECHNOLOGY AND NANOAGRICULTURE

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ABSTRACT

Chitinases are enzymes that catalyze the degradation of β-1,4-linkages in chitin, the second most abundant polymer on earth, after cellulose, generated from the cell walls of fungi, shells of crustaceans and cuticles of insects. Chitinases have been detected in many organisms including bacteria, fungi, insects, plants, mammals and human. These enzymes are highly preserved through species and have various functions in many living organisms. For instance, in yeast and fungi chitinases participate in morphogenesis, in plants have an important role against pathogens, and in insects are implicated in the processes of development and growth, during ecdysis. Chitinases are widely used in research and industrial applications. In food industry are used for extraction of chitin and chitosan or digestion of seafood shells. In agriculture, chitinases are used as biological control agents that cleave chitin and protect hosts against pathogens. Chitinases from human body are important markers in detection of allergies, asthma, cancer and Gaucher disease. The acidic mammalian chitinase, show high catalytic activity at pH 2 and is expressed in gastric epithelia, in lung macrophages and in the pulmonary epithelia during asthmatic inflammation. In addition, new applications appear in nanobiotechnology field, where chitinases are used as enzymes which contribute at biosynthesis, stabilization or degradation of different types of nanoparticles. Biogenic formation of nanosilver or nanogold using microorganisms or biologically active metabolites such as enzymes (chitinase, amylase, protease, catalase, nitrate reductase and tyrosinase), peptides, organic acids, antimicrobial metabolites, is an efficient, green and fast way for production of nanoparticles. Interactions between nanoparticles and proteins lead to the stabilization and the formation of nanoparticle-biomolecular-capped structures with anticancer properties. Silver nanoparticles have higher affinity for chitinase than for other synthetic substrates and played a major role in the thermal stability of chitinase. In this work, the antibacterial and antifungal effect of a chitinase is showed. Moreover, the biosynthesis

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and stability of silver nanoparticles using a recombinant chitinase produced by *Escherichia coli* is under analysis.

Keywords: chitinase, chitosan, nanoparticles, protein corona

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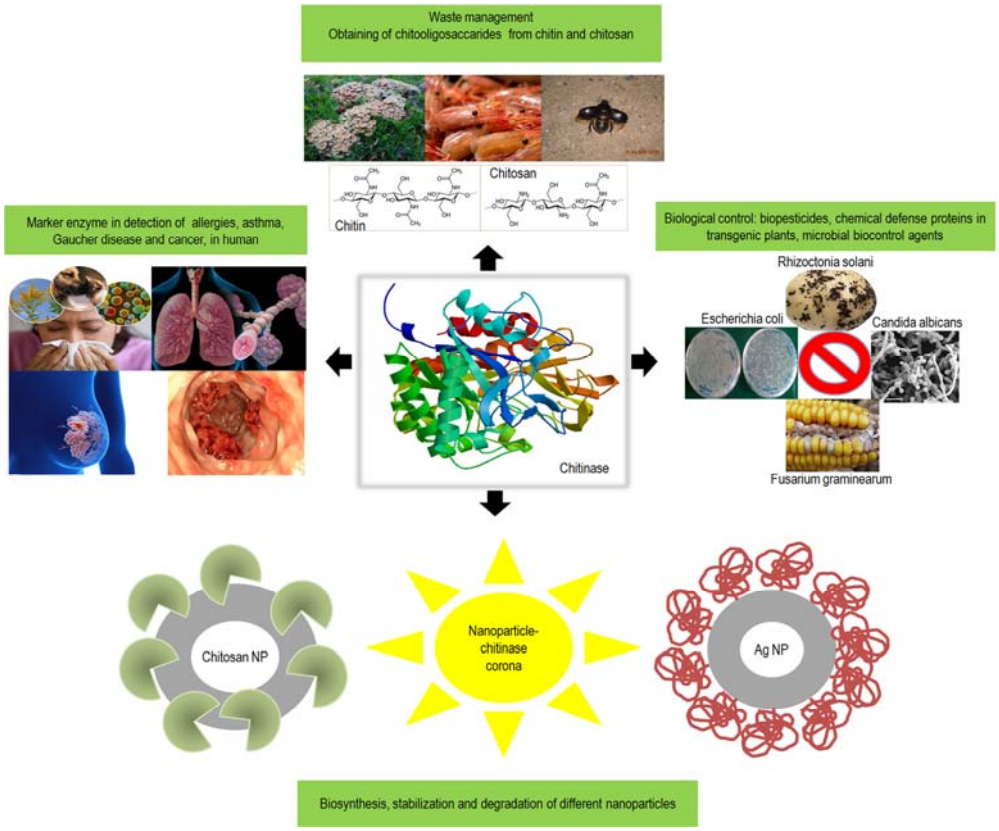
ABSTRACT FIGURE



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Abstract/Graphical Abstract

MEDICAL TRANSLATION BETWEEN ACCURACY AND IMPOSTURE

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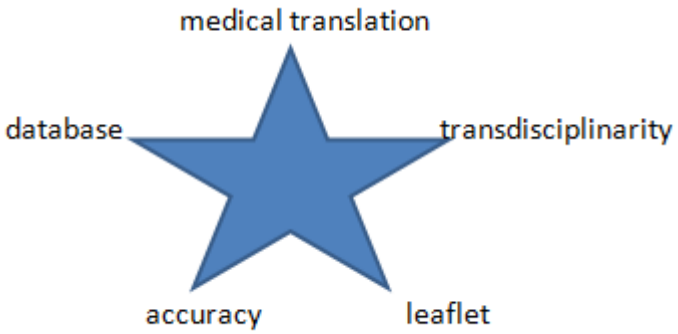
ABSTRACT

Globalization means, among many other effects, an increase in the number of imported products, especially in the medical field. As a result of this phenomenon, the demand for translations of medical prospectuses has become enormous.



Translators are either medical specialists or language specialists. The first are qualified in the medical field, plus they have translation skills or they know a foreign language. Others choose this profession as a result of their linguistic skills and then they specialize in the medical area.

Pharmaceutical companies are always looking for collaborators specialized in both linguistic and medical fields.

The accuracy of a leaflet translation, of a medicine approval file, of a medical record, of a clinical trial has enormous implications for patients and for professionals, and is therefore absolutely mandatory. "Keep this leaflet. You may need to read it." is a warning that emphasizes the importance of that paper that we find in all medicine boxes. Theoretically, it should guard us against any danger associated with the use of that medicine. The problem is that the language used in this area is far from being unitary, that terms are often translated at random and that we sometimes find meaningless phrases.

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That is why we are proposing to present some samples of prospectuses on the idea that greater efforts should be made to build linguistic databases for the medical field. Informatics, linguistics and, last but not least, pharmaceutical science should work inter- and transdisciplinary to avoid arbitrary errors and expressions. Only by working in multidisciplinary teams useful results for all actors involved will be obtained, in production, recommendation and consumption of medicines.

Keywords: medical translation, leaflet (prospectus), accuracy, database.

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NANO-MOD **2019**
22-23 April, Timişoara
*NEW FRONT CHEM 28 (**2019**) 1-66*

Abstract/Graphical Abstract

PRELIMINARY STUDIES ON CHITOSAN BASED MEMBRANE COMPOSITES

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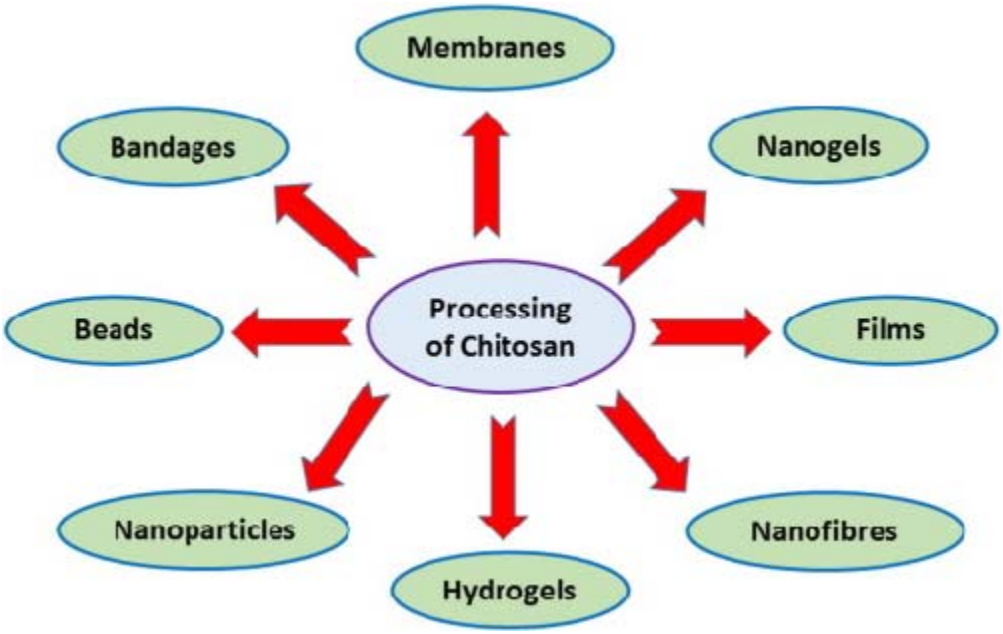
ABSTRACT

Chitosan is an important and abundant biopolymer material with numerous applications in various different fields, due to its antimicrobial activity, low toxicity, biodegradability, biocompatibility, mechanical characteristics and stabilization capability [1,2,3]. Chitosan structure, consisting of glucosamine and N-acetylglucosamine units, determines its properties [4]. It can be used in different forms i.e. beads, films, coatings, fibers or sponges. Recently, chitosan-based membranes are being intensively studied for wound healing applications due to easy fabrication and aforementioned properties. Literature data revealed that higher molecular weight chitosan present good film-forming properties caused by intra- and inter molecular hydrogen bonding [5].
In order to evaluate how the membranes physicochemical properties are influenced by the chitosan molecular weight and the type of substance added during the dissolution of the chitosan, four different types of films containing 2% chitosan, 2% chitosan and glycerol, 2% chitosan and zeolite and 2% chitosan with glycerol and zeolite were prepared [3,6]. Transparent and flexible chitosan membranes were obtained from chitosan with three different molecular weights (MW 50 – 1000, 300 – 2000, 500 – 5000 kDa).
This preliminary study showed that chitosan molecular weight is an important parameter that should be considered when different membranes, for various uses, are prepared.

Keywords: biomaterials, nano-biomimetic materials, chitosan.

ABSTRACT FIGURE



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Abstract/Graphical Abstract

PREDICTION OF THE PHARMACOLOGICAL PROFILES OF SOME OLIGOMERS OF LACTIC ACID. A COMPUTATIONAL STUDY. ††

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ABSTRACT

Poly-L-lactic acid (PLLA) is one of the most promising biobased and biodegradable polymers used in packaging [1] and for biomedical applications (drug delivery systems, degradable sutures, and porous scaffolds) [1, 2]. There are a few known side effects of PLLA on humans, such as allergic reaction, angioedema, hypersensitivity reactions [3]. We have considered oligomers containing from 1 to 16 units of lactic acid and have predicted their pharmacokinetics profiles and toxicological endpoints using SwissADME tool [4]. Our findings reveal favorable pharmacokinetics profiles of the oligomers of PLLA: they do not inhibit the human cytochromes involved in the metabolism of xenobiotics, do not reflect hepatotoxicity, mutagenicity, and carcinogenicity and their skin penetration coefficients decrease with increasing molecular weight. The following adverse effects are predicted: a weak potential of cardiotoxicity by inhibition of the h-ERG channels, the potential of eye irritation and corrosion, especially for smaller molecular weight oligomers.

Keywords: polylactic acid, pharmacokinetics, toxicity.

†† This work was supported by Grant: PNIII-P3-285 Polymeric NanoBioMaterials for drug delivery: developing and implementation of safe-by-design concept enabling safe healthcare solutions – GoNanoBioMat
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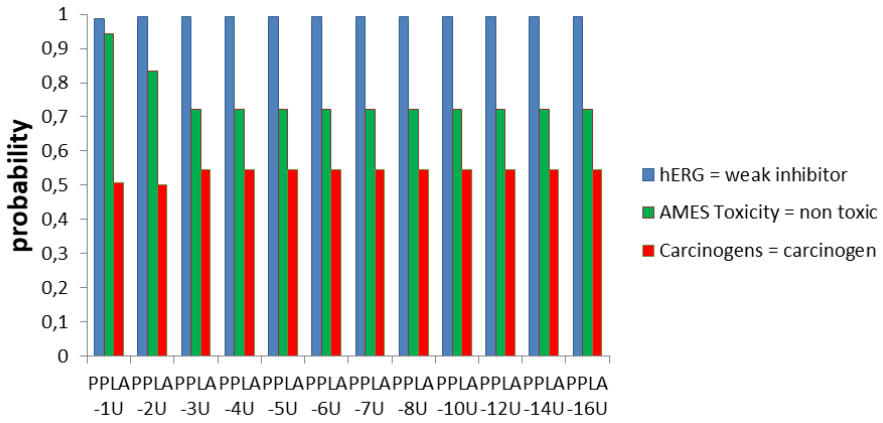
ABSTRACT FIGURE



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NANO-MOD **2019**
22-23 April, Timişoara
*NEW FRONT CHEM 28 (**2019**) 1-66*

Abstract/Graphical Abstract

THE INFLUENCE OF ORGANIC STABILIZATORS IN THE WATER SPLITTING PROCESS USING SEMICONDUCTOR PHOTOCATALYSTS

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ABSTRACT

Taking into account the current environmental pollution level, development of renewable and eco-friendly technologies have priority over the old ones involving fossil fuels and other materials with toxic waste by-products [1]. A good example of alternative energy source is environmentally friendly hydrogen which is obtained from other renewable resources, sunlight and water [1,2]. This technique involves a process called water splitting which takes place in very particular conditions, requiring specific band gap, valence band and conduction band values, low photo-corrosion affinity, efficient separation of photo-generated electrons and holes in semiconductors, and the most important, activity of the photocatalysts under visible light, which is also a major part of this research [3].

In the present, most studied materials in this field are sulfides, due to their high activity under visible light [4]. Unfortunately, this ability undergoes recombination of photogenerated electron-hole pairs, which can be decreased by the introduction of organic stabilizators. Graphene and its derivatives, graphene oxide (GO) and reduced graphene oxide (rGO), have been used in many applications [2], their high performance being also observed in the graphene-based photocatalysts [5]. Effectiveness of the graphenic materials in the photocatalytic process is mainly due to their high surface area and excellent charge transport [6,7], properties that are linked to their zero band gap, this way contributing to the adsorptive, charge separation and transportation abilities of the graphene-semiconductor composite materials.

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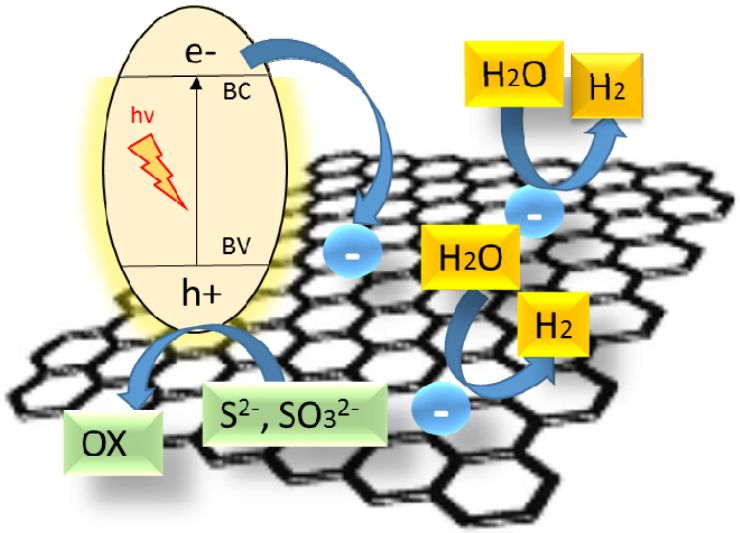
Keywords: photocatalysts, water splitting, graphene oxide.



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Abstract/Graphical Abstract

OPTIMIZING DEVICE OF LOGICAL MATRICES TOWARDS SEMICONDUCTIVITY

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ABSTRACT

Since its discovery, graphene along with the previously existent carbon allotropes have become part of multiple technologies and composite materials [1]. The properties of graphene include mechanical strength, superior thermal conductivity, transparency, high specific surface area, and excellent charge transport [2,3]. Good conductivity of the graphene can be attributed to the position of p orbitals which result in delocalized ☐ bonds moving freely in the whole graphene plane [4]. As a consequence, high conductivity of graphene could be explained by the presence of zero-energy band gap. More precisely, the place where π*-state conduction band (CB) and the π-state valence band (VB) touch each other result in Dirac point [5].

The ambivalent nature of graphene ca be demonstrated by the introduction of foreign atoms and defect sites on the lattice of graphene which highly influence its electrical properties [6,7], resulting in a p-type or an n-type semiconductor [8].

A tunable band gap however, could be obtained from insulating to conducting by controlling the reduction degree of rGO, as the band gap energy is strongly correlated with the number of oxidized sites, and the oxidization degree of rGO [9].

In this work the aim was to study the graphene-oxide/TiO_2 semiconductors with tunable conductivity, placed in a specific matriceal sequence, in order to predict a conductivity pattern based on quantic effects that take place. It is presumed that the non-contact depositions placed at micrometric distances will induce new interactions.

Keywords: semiconductor, graphene, logical matrices.

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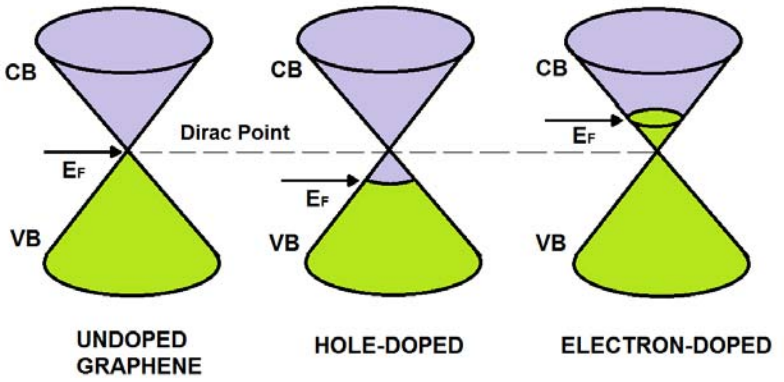

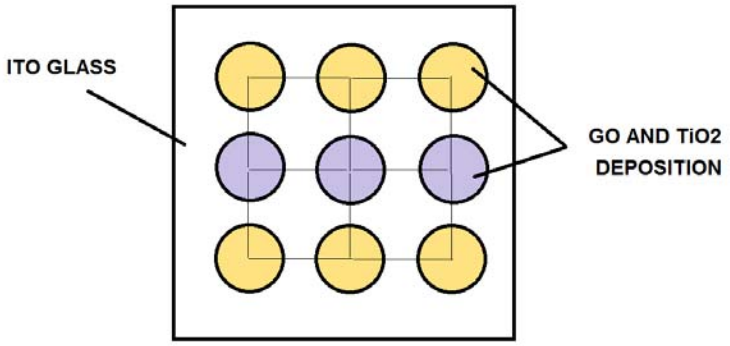

ACKNOWLEDGEMENT

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NANO-MOD **2019**
22-23 April, Timişoara
*NEW FRONT CHEM 28 (**2019**) 1-66*

2nd Nano-Modeling of Strategic Materials for Knowledge Economy
Book of Abstracts

Abstract/Graphical Abstract

CHEMICAL REACTIVITY DRIVING SWITCHABLE MOLECULAR MACHINES

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ABSTRACT

Supramolecular chemistry, an attractive field of chemistry that studies the chemical systems composed of assembled molecular subunits like molecular machines. This young field of chemistry is the way to development of new nanodevices and nanotechnologies [1-4]. Calixarene-based rotaxanes is a class of complexes intense tested as mechanically interlocked molecular architectures and molecular machines (they can make molecular motions e.g.: rotation motions, translation motions) [5-7]. Slipping method is one of the principal routes used for rotaxane synthesis (Figure 1) [8-10]. At high temperature the dumbbell (axle of rotaxane) reversibly thread through the macrocycle (the ring/wheel of rotaxane) and when the mixture is cooled, the thread/axle is stuck in the macrocycle and the rotaxane cannot deslip[8-10]. Deslipping is the reverse process of the slipping. [8-10]. The molecular structure has proven to include the key pathway towards chemical reactivity [11-17]. In these study we used the chemical reactivity indices: electronegativity (χ), chemical hardness (η), chemical power index (π), electrophilicity (ω) and their principles (electronegativity and its minimizing principle, followed by chemical hardness maximization, then followed by minimum activation - chemical power index (π), electrophilicity (ω)) [11-17]. With these indices we try to establishes hierarchy for chemical interaction scenario [18,19] during the motion of the rotaxane-based molecular machine and also during the slipping/deslipping process (synthesis of the rotaxane-based molecular machines).The calixare-based rotaxane complexe under this study is MMC (Figure 2). This molecular machine complex (MMC) contain as wheel tris(N-phenylureido)-calix[6]arene and as axle a 4,4'-bipyridinium dication units, is deeply encapsulated within the wheel and not affected by the solvent polarity. Similar approach may be also taken also for the structure of rotaxane $9H^{3+}$ (initial, transient and final) and the processes that take place during its operation as a pH-controllable

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molecular shuttle (Figure 3), in what can be called as ACID-BASES Switchable Molecular Machines [20].

Keywords: Molecular machines, Rotaxane, Calixarene, Chemical reactivity indices.

ABSTRACT FIGURES

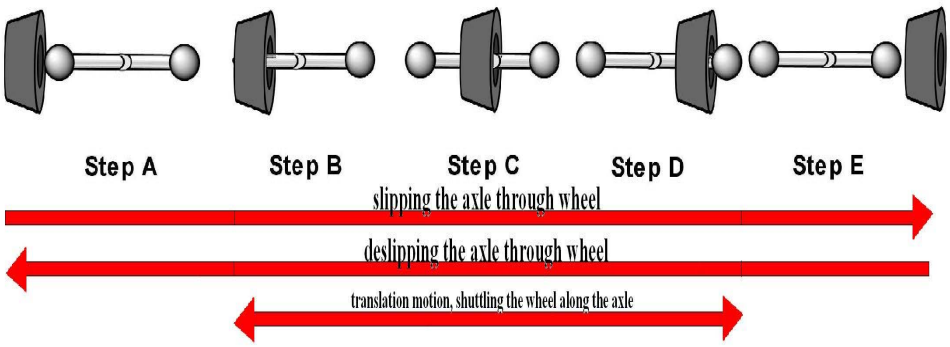

Figure 1. Slipping/deslipping process in a rotaxane synthesis, translation motions in a rotaxane-based molecular machine

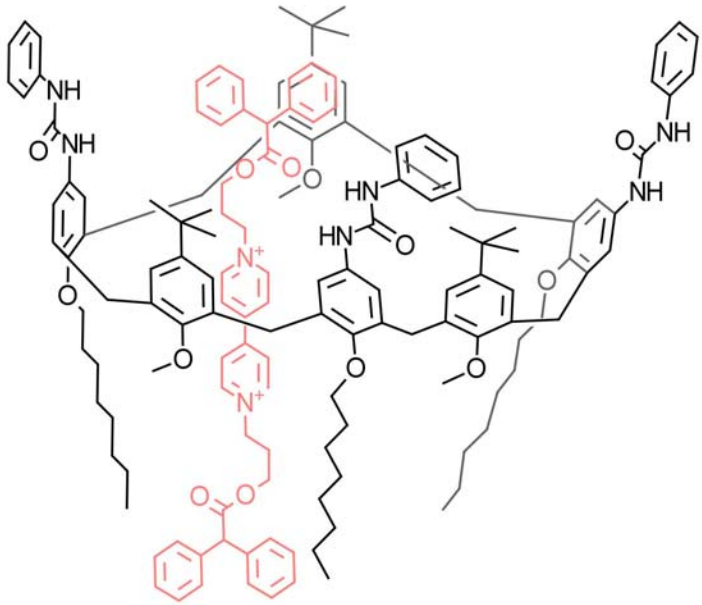

Figure 2. Calixarene-based rotaxane MMC which contain as wheel tris(N-phenylureido)-calix[6]arene and as axle a 4,4'-bipyridinium dication unit

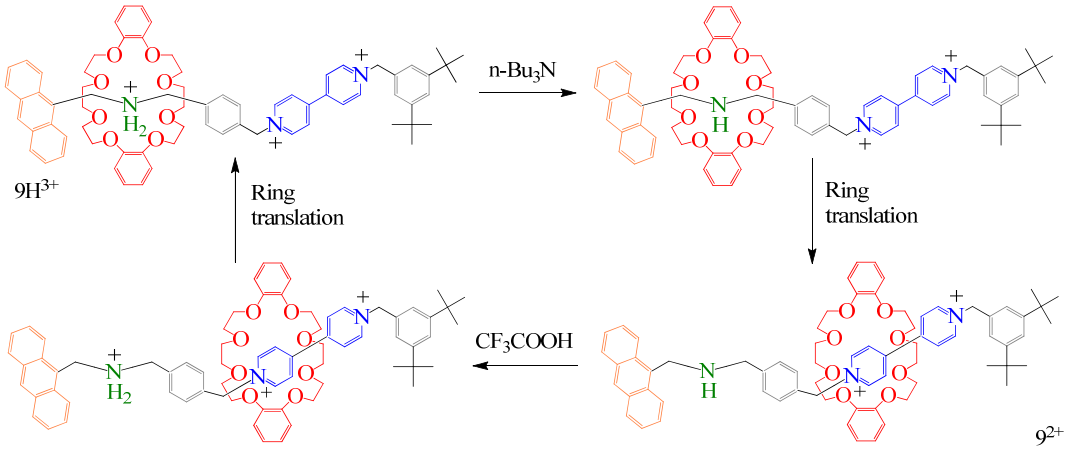

Figure 3. The formula of rotaxane $9H^{3+}$ structure and the representation of its operation as a pH-controllable molecular shuttle.

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2nd Nano-Modeling of Strategic Materials for Knowledge Economy
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GREEN'S FUNCTION IN MODELING GRAPHENIC CHEMICAL BONDS

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ABSTRACT

Graphene has attracted a lot of attention in the last years due to its physical and mechanical properties, being stronger than steel, very light and very flexible, having high thermal and electronic conductivities [1]. In general, one can define graphene as a carbon allotrope arranged in a stable hexagonal lattice with sp2 orbital hybridization and 0.34 nm thickness (corresponding to one atom of carbon). On the other hand, Green's Function can be viewed as important tool in quantum mechanics with different application, such as: determining the values for density of states, eigenfunction and eigenenergies [2], describing the propagation of a one-particle or one-hole in a medium, transport calculation or in modelling, the arbitrary geometries or the scattering processes belonging to the single-particle approximation for graphene. From the classical field perspective, Green function can be constructed by considering in the filed strength, at one specific point, the contribution out of a unit source from another specific point [3].

$$\phi(x) = \int G(x,x')J(x')d^4x' \quad (1)$$

In second quantized theories of systems with many particles, the Green function is of the form [3]:

$$G(x,x') \equiv \lim_{J\to 0} \frac{\delta\langle\partial\phi(x)\rangle}{\partial J(x')} \quad (2)$$

The Green's function can be also constructed starting from two Dyson formula (3) and (4),

$$G = G^{(0)} + G^{(0)}VG \quad (3)$$

$$G = G^{(0)} + GVG^{(0)} \quad (4)$$

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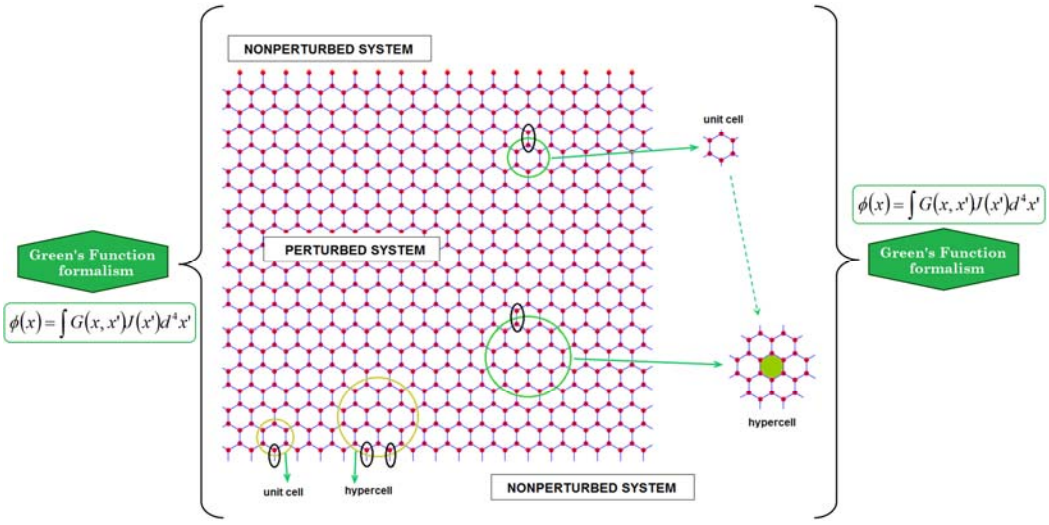
leading to a recursive relations for a system quasi-one-dimensional which is coupled to leads [4]. This algorithm is based on breaking the system into independent leads and slices, to which are associated "unperturbed" Green's functions $G^{(0)}$; the perturbation V is used to build selectively the hoping matrix elements which connects the parts. As for the disordered graphene [5], the most common model used in describing its electronic transport is considered to be the effective low-energy Dirac Hamiltonian which is combined with an expression of the standard diagrammatic perturbative type. In practice, one can also address the two-/multiple-probe conductance while considering the geometry of the studied system; in this context, the recursive Green's function [6] become appropriate in order to compute the transport properties of the respective systems.

Keywords: Green's function, graphene, quantum mechanics, eigenfunction, eigenenergies.

ABSTRACT FIGURE



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Abstract/Graphical Abstract

ASSESSMENT OF THE HUMAN HAZARD OF SOME OLIGOMERS OF POLYHYDROXYALKANOATES ‡‡

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ABSTRACT

Polyhydroxyalkanoates (PHAs) are natural polymers produced by various microorganisms. Due to their biocompatibility and biodegradability, PHAs have numerous biomedical applications [1]: drug delivery systems, bone and cartilage regeneration, vascular system devices and wound management. It is also well known that exogenous ketone supplements are frequently used by those intending to lose weight and to increase exercise performance. [2]. There are various congeners of PHAs, but short chain length polymers such as poly-3-hydroxybutyrate (P3HB), poly-3-hydroxyvalerate (P3HV), poly-4-hydroxybutyrate (P4HB), poly-4-(hydroxyvalerate) and their copolymers are largely used in therapeutic applications [3]. Due to the autocatalytic degradation of these polymers, small oligomers are released in the human body. Within this study, we have used a computational approach to assess the pharmacokinetic profiles of small oligomers of 3-hydroxybutyrate, 3-hydroxyvalerate, 4-hydroxybutyrate, 4-hydroxyvalerate, and their co-oligomers. The outputs of our study suggest that investigated small oligomers have favorable pharmacokinetic profiles revealing good bioavailability, are not potential inhibitors of human cytochromes involved in drug metabolism, are not carcinogen and mutagen. The investigated oligomers are possible inhibitors of organ anion transporters OATP1B1 and OATP1B3, which may influence the absorption of some drugs in the liver and smaller molecular weight oligomers can cause eye irritation.

Keywords: polyhydroxyalkanoates, pharmacokinetics, toxicity.

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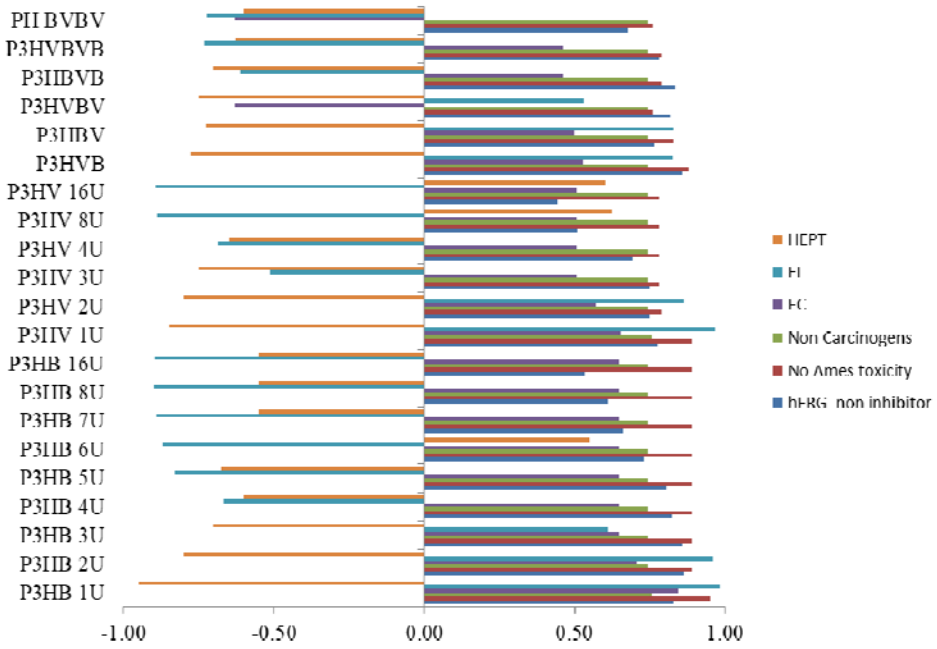
ABSTRACT FIGURE



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Abstract/Graphical Abstract

LD/MM+ SIMULATION OF SOME COUPLED SPECIES IN BOX WATER

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ABSTRACT

The aim of this study was to understand the dynamics interactions of some coupled species with humic and aristolochic acids, in water box, using Langevin Dynamics (LD) [1] simulation method, and molecular dynamics mechanism (MM+) [2], because these methods can fold extended sequences to `global' potential energy minima for very small systems (peptides of length ten, or so, in vacuum), but it is most commonly used to simulate the dynamics of known structures [3] and the jostling of a solute by solvent can expedite barrier crossing, and hence Langevin dynamics can search conformations better than Newtonian molecular dynamics.[4]

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We used in this paper aristolochic acids,because they are a mixture of structurally related nitrophenanthrene carboxylic acids, carcinogenic and nephrotoxic agents. This study is one of the molecular docking that presents the interactions between a molecular model of the humic acid structure and 18 aristolochic acids structures from PubChem database in a water box that simulates the environment reactions. (PubChem, 2018). [5,6]
This study reviews numerical simulations of quantum field theories based on stochastic quantization and the Langevin equation. The topics discussed include renormalization of finite step-size algorithms, Fourier acceleration, and the relation of the Langevin equation to hybrid stochastic algorithms and hybrid Monte Carlo.[1,7,8,9,10]
From the values obtained, calculated by function optimization in a numerical analysis [8], the binding energy that is the minimum energy required to disassemble the entire system in separate parts, have achieved a system that has less potential energy than the sum of its components.
We have three results that were eliminated from the analyze algorithm ,those of the 17.18 and 19 components, because cannot succesed to finished the optimization, because of the restricted limitation of cicles in the HyperCHEM program. [6]

Keywords: LD/MM+; humic substances

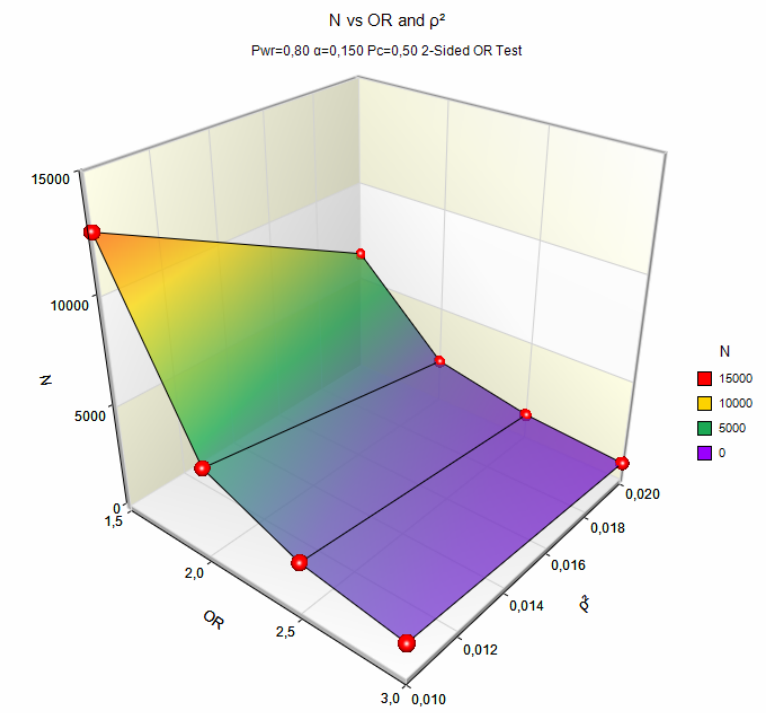

Figure 1. *The plot of the probability between kinetic and potential energy*

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