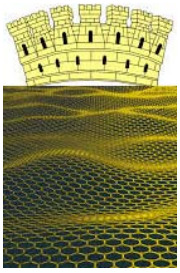


NEW FRONTIERS IN CHEMISTRY
New Front. Chem.

(*former Annals of West University of Timişoara – Series of Chemistry*)

(2018) Volume 27, Number (Issue) 1, pp. 1-49

Special Issue Dedicated to

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

16 –17 May 2018, Timişoara

&

Green nanochemistry - application of the safe by design principle for obtaining new nanomaterials

7 June 2018, Timişoara

TABLE OF CONTENTS

PUBLISHER:
Universitatea de Vest din Timişoara

NEW FRONTIERS IN CHEMISTRY: METADATA

New Frontiers in Chemistry (New Front. Chem.) is an open-access fee-free peer-review international academic journal addressing the modern trends and frontiers in fundamental, applicative and multidisciplinary chemistry, paralleling the ever-expanding chemical data, methods, and compounds available and continuously produced, towards cross fertilizing the multidisciplinary ideas as coming from Chemistry combined with Mathematics, the Natural and Applied sciences (Physics, Biology, Medicine, Agriculture, Environmental, Engineering), and beyond.

NEW FRONTIERS IN CHEMISTRY
(NEW FRONT. CHEM.)
is published biannually by

West University of Timișoara
Blvd. V. Parvan 4
Timisoara 300223, ROMANIA
E-mail: newfrontchem@iqstorm.ro
Web: www.newfrontchem.iqstorm.ro

ISSN 2393 – 2171
ISSN-L 2393 – 2171

Subscription Price per Volume
Electronic: open access Print: on demand by above email address

Additional color graphics is available in the e-version of this Journal

NEW FRONTIERS IN CHEMISTRY: EDITORS

Editorial Board:

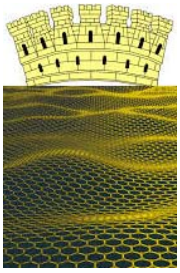
NEW FRONTIERS IN CHEMISTRY:

PROCEEDING OF ABSTRACTS

Nano-Modeling of Strategic Materials for Knowledge Economy
(NANO-MOD)
16 –17 May 2018, Timişoara

Editor:

MIHAI V. PUTZ
West University of Timişoara
Faculty of Chemistry, Biology, Geography
Biology-Chemistry Department
Timişoara, ROMANIA



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

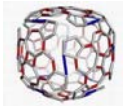
Timișoara (2018) 16-17 May

Research Workshop
First Edition

SUPPORTED BY:

West university of Timișoara: Faculty of Chemistry, Biology, Geography, Faculty of Economics and Business Administrations, Laboratory of Structural and Computational Physical-Chemistry for Nanosciences and QSAR, Laboratories of Advanced Environmental Researches

National R&D Institute for Electrochemistry and Condensed Matter: Laboratory of Renewable Energies - Photovoltaics



European Society of Mathematical Chemistry

PROGRAM & BOOK OF ABSTRACTS

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 2018

LOCATION:

West University of Timisoara, Pestalozzi Str. No. 16 B (300115 Timisoara)

https://www.google.ro/maps/@45.7533937,21.2420762,17.97z

The P02 (ground) Hall & Lounge of FEAA

(Faculty of Economy & Business Administration)

DISSEMINATION:

Special Issue of *New Frontiers of Chemistry*

http://www.newfrontchem.iqstorm.ro/

CHAIR:

Mihai V. PUTZ

(Phone: 0726-011-866; Fax: 0256-592-620; E-mail: mihai.putz@e-uvt.ro)

COMMITTEE:

Corina DUDA-SEIMAN (Executive Organizer)

Vasile OSTAFE (Biology-Chemistry Department Director)

Mircea SELEGEAN (Guest Matters)

Mircea DIUDEA (ESMC & IAMC President)

Ottorino ORI (Scientific Secretary)

Marius MIRICA, Mirela IORGA, Doru BUZATU (INCEMC-Timisoara)

NANO-MOD 2018: PROGRAM & ABSTRACTS

		Oral Presentations (P02Hall@FEAA**)**:	
16 May 2018	10-10.30	Mihai V. Putz *(West University of Timişoara)*	*Opening & Memento Prof. Dr. A. Chiriac*
(*Chairman*: Prof. Dr. V. Ostafe)	10.30-11	Mihai V. Putz & Ioan Petrisor *(West University of Timişoara)*	*Multidimensional clustering and multi-scientific emergings*
	11-11.30	Ana Maria Toader & Fanica Cimpoesu *(Physical-Chemistry Institute "Ilie Murgulescu" of Romanian Academy)*	*Back to the basis! Reforming elements of computational chemistry*
	11.30-12	Lorentz Jäntschi & Sorana D. Bolboacă *(Technical University of Cluj-Napoca & University of Medicine and Pharmacy Cluj-Napoca)*	*Computational study on six linear homopolymers: are their helical structures stable?*
	12AM-13PM	**Break for Brunch (Lounge@FEAA)**	
16 May 2018	13-13.30	Claudiu N. Lungu et al. *(Babes-Bolyai University)*	*Magnetic nanoparticle explored for bioactive molecular manodevice*
(*Chairman*: Prof. Dr. L. Jantschi)	13.30-14	Lorentz Jäntschi et al. *(Technical University of Cluj-Napoca)*	*I have the geometry but I lost the way of arriving to it; what I have to do?*
	14-14.30	Bogdan Bumbacila et al. *(West University of Timişoara)*	*New approaches clinical studies of anticancer in pre-drugs*
16 May 2018	18-21	**Guest Research Workshop Dinner (location to be announced to the participants, *in situ*)**	
17 May 2018	10-10.30	Adriana Isvoran et al. *(West University of Timişoara)*	*Molecular weight dependence of ADME-Tox properties of chitin and chitosan oligomers*
(*Chairman*: CS1 Dr. F.Cimpoesu)	10.30-11	Ana-Maria Putz et al. *(Timişoara Institute of Chemistry of Romanian Academy)*	*Drug delivery systems*
	11-11.30 (Last Entry)	Duda-Seiman D. et al. (*University of Medicine and Pharmacy Timişoara*)	*Smoking and stress – the new old enemies*
	11.30-12	Mihai V. Putz, Fanica Cimpoesu, & Marilena Ferbinteanu *(West University of Timişoara, Physical-Chemistry Institute "Ilie Murgulescu" of Romanian Academy, & University of Bucharest)*	International TextBook Presentation*: Structural Chemistry: Principles, Methods and Case Studies* (Springer Verlag 2018)
17 May 2018	12AM-14PM	**Break & Poster Presentations (Lounge@FEAA) ~ see below ~**	

Posters' Presentations (Lounge@FEAA**)**:		
17 May 2018 (12AM-14PM)	Ana M. Toader et al. *(Physical-Chemistry Institute "Ilie Murgulescu" of Romanian Academy)*	*On the electronic structure of triangular polyaromatic hydrocarbons with Spin*
	Cristina M. Buta et al. *(Physical-Chemistry Institute "Ilie Murgulescu" of Romanian Academy)*	*Structural analyses of interacting nitroxide-based organic radicals.*
	Alice Mischie et al. *(Physical-Chemistry Institute "Ilie Murgulescu" of Romanian Academy)*	*Revisiting ring strain with combined quantum techniques*
	Vasile Simulescu & Gheorghe Ilia *(Timişoara Institute of Chemistry of Romanian Academy)*	*Organic- hybrids containing phosphorus compounds inorganic*
	Mirela I. Iorga et al. *(National R&D Institute for Electrochemistry and Condensed Matter)*	*Quantum electrochemical systems and Machines*
	Doru L. Buzatu et al. *(National R&D Institute for Electrochemistry and Condensed Matter)*	*The present future of the graphenic semiconductor*
	Daniela Dascălu et al. *(West University of Timişoara)*	*Correlation of chemical bonds orders calculated by molecular orbitals method with some properties of simple and complex substances*
	Roxana Nicola et al. *(Timişoara Institute of Chemistry of Romanian Academy)*	*Synthesis and characterization of iron oxide nanoparticles coated with mesoporous silica via surfactant template sol-gel method. Influence of CTAB/SiO2 ratio upon morpho-textural properties*
	Mirela Picioruş et al. *(Timişoara Institute of Chemistry of Romanian Academy)*	*Template free spherical silica. Role of precursor in Stoeber Synthesis*
	Ana-Maria Udrea, Alin Puia et al. *(University of Bucharest)*	*Melatonin, Resveratrol, Linalool and Linalyl Acetate - new perspectives in treatment of depression*
	Diana L. Roman et al. (*West University of Timişoara*)	*Prediction of ADME-Tox properties of polylactic acid oligomers*

Abstract/Graphical Abstract

MULTIDIMENSIONAL CLUSTERING AND MULTI-SCIENTIFIC EMERGINGS

Mihai V. PUTZ
West University of Timișoara, Faculty of Chemistry - Biology Geography & Doctoral School of Economics and Business Administration; National Institute for R&D in Electrochemistry and Condensed Matter –Laboratory of Renewable Energy-Photovoltaics, Timișoara, ROMANIA
Email: mv_putz@yahoo.com, mihai.putz@e-uvt.ro

Ioan PETRIȘOR
West University of Timișoara, Faculty of Economics and Business Administration, Timișoara, ROMANIA
Email: ioan.petrisor@e-uvt.ro

In the context of globalization and networking, the new concept of cubic clustering is advanced, within the multi-generational hierarchy as emerging of the nano-scientific and nano-technological society evo/devo-lution:

1. the 1D level specific to the clustering germination (…modeling by crystallography)
2. the 2D level specific to the clustering fractals (transforming the non-regularities in regularities at large, while imposing the standards, rules and protocols in various economical fields, industries, disciplines, societies, etc.)
3. the 3D level specific to cubic clustering, marking the emerging of networking, with all consequences (to be discussed);
4. the 4D level specific to digital (also quantum) clustering, emphasizing on multi-dimensionality, coding-decoding of information and strategies, at both local and global (virtual clusters) manifestations.

Keywords: strategic management, cubic management, clustering, nano-technology, knowledge economy.

NANO-MOD **2018**
16-17 May, Timișoara
West University of Timișoara
*NEW FRONT CHEM 27 (**2018**) 1-36*

Abstract/Graphical Abstract

BACK TO THE BASIS! REFORMING ELEMENTS OF COMPUTATIONAL CHEMISTRY

Ana Maria Toader and Fanica Cimpoesu*

Institute of Physical Chemistry, Splaiul Independentei 202, Bucharest 060021, Romania

The computational chemistry is a distinct branch of modern fundamental chemistry and at the same time a valuable counterpart of the applied material sciences, providing valuable explanations and predictions as guidelines for achieving desired properties. The vast majority of quantum chemical calculations is based on the so-called Gaussian Type Orbitals (GTOs), which represent the "concrete and steel" of the actual development in this field. [1] A hidden drawback, overlooked by the quasi-unanimity of users and developers of quantum chemistry programs, stays in the fact that the standardized GTO bases have drastic limitations in the radial polynomial co-factors.[2] Thus, all the GTOs for a shell with l quantum number are only collections of $r^l\exp(-\alpha r^2)$ terms. We alleviate this situation introducing general $r^k\exp(-\alpha r^2)$ primitives, in analogy to known exact solutions for hydrogen case. Thus, in spite of the tacit belief that all the methodological backgrounds are nowadays clarified, it seems that revolutions are yet possible.

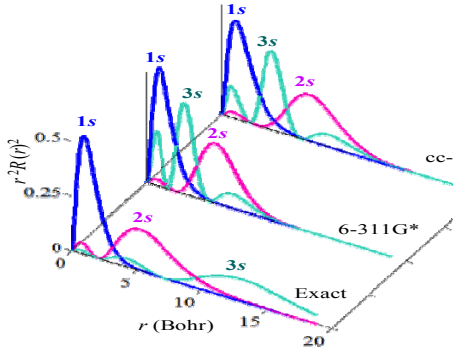


Fig.1 Illustration of hidden drawbacks of current GTOs on hydrogen atom cases. The wrong account of superior quantum numbers.

n	Correct Energies	Gaussian cc-	Improved Gaussian
1	-0.5	-0.49999	-0.499940246
2	-0.125	-0.072873	-0.124911031
3	-0.05555	0.52548	-0.055446687
4	-0.03125	2.5213	-0.031104313
5	-0.02	11.922	0.175969578
6	-		1.432637114
7	-		6.220137647
8	-		27.57288979
9	-		129.830686
1	-0.005		790.7138151

References.

[1]F. Jensen, *Introduction to Computational Chemistry*, John Wiley & Sons Ltd, Sussex, 2007.

[2] M. V. Putz, F. Cimpoesu, Marilena Ferbinteanu ,*Structural Chemistry. Principles, Methods, and Case Studies*, Springer, 2018.

NANO-MOD **2018**
16-17 May, Timişoara
West University of Timişoara
*NEW FRONT CHEM 27 (**2018**) 1-36*

Abstract/Graphical Abstract

COMPUTATIONAL STUDY ON SIX LINEAR HOMOPOLYMERS: ARE THEIR HELICAL STRUCTURES STABLE?

Lorentz JÄNTSCHI[1,2] **and Sorana D. BOLBOACĂ**[3]

[1] Department of Physics and Chemistry, Technical University of Cluj-Napoca, 400641 Cluj-Napoca, Romania. E-mail: lorentz.jantschi@gmail.com
[2] Chemistry Doctoral School, Babeş-Bolyai University, 400028 Cluj-Napoca, Romania
[3] Department of Medical Informatics and Biostatistics, Iuliu Haţieganu University of Medicine and Pharmacy, 400349 Cluj-Napoca, Romania. E-mail: sbolboaca@umfcluj.ro

Background: Polymers are macromolecule composed of many repeated monomers. The biopolymers such as DNA (**D**eoxyribo**N**ucleic **A**cid) and proteins are naturally organized as helical structures with precise structural and functional properties. Hypothesis: The helical structure is valid also for homopolymers.

Aim: Our study aimed to investigate if six linear chained homopolymers likely to have a helical structure can stabilize as a helix and if yes to identify the parameters of the helix.

Material and method: Six homopolymers have been used in this computation study:

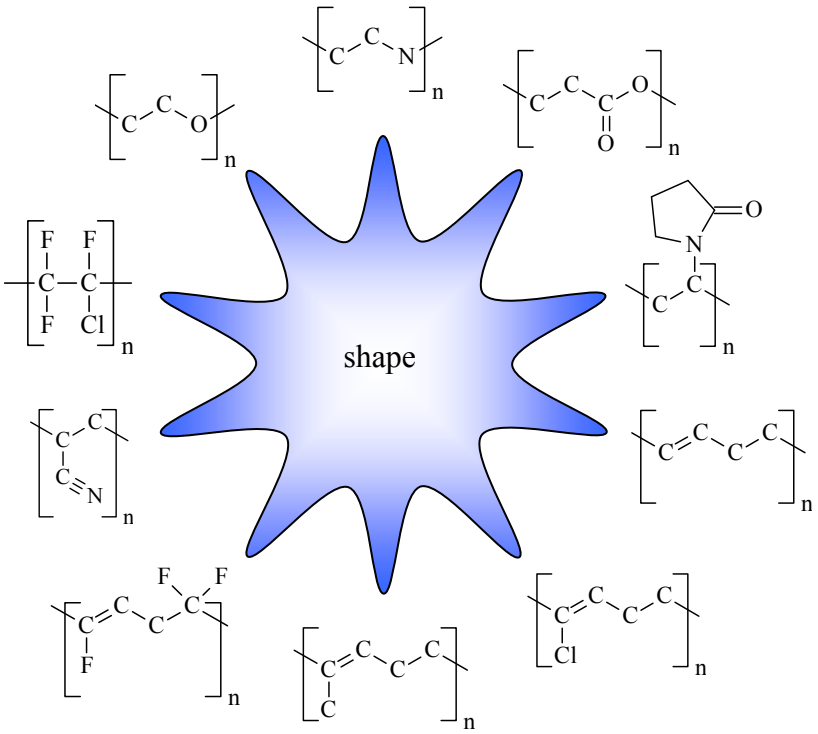
Name	**Formula**	**Utility**
poly(lactic acid)	$(C_3H_4O_2)_n$	biocompatibility and dissolvability in the body → tissue engineering, delivery systems
poly(1-chloro-trans-1-butenylene)	$(C_4H_5Cl)_n$	
poly(1-methyl-trans-1-butenylene)	$(C_5H_8)_n$	
poly(1,4,4-trifluoro-trans-1-butenylene)	$(C_4H_3F_3)_n$	
polyacrylonitrile	$(C_3H_3N)_n$	hard, relatively insoluble, and a high-melting material → carbon fibers, nanofibers, microcapsules/microspheres with diverse application
polychlorotrifluoroethylene	$(CF_2CClF)_n$	nonflammable, high optical transparency, chemical resistant, has near-zero moisture absorption, and excellent electrical properties → packaging (pharmaceutical and medical industry)

The polymers with seventeen (poly(lactic acid)) or eighteen monomers (all others) were drawn with HyperChem software. The geometries of the resulted polymers were optimized with

Spartan program (Hartree-Fock 6-31G* level of the theory). X, Y, and Z coordinates and the best guest value of the coefficient of the helix (obtained by inspection of the graphical representations of the optimized polymers) were the input data used to identify the optimal values of the helix coefficients by minimizing the residuals.

Results: The calculated coefficients of the helixes had, with one exception (poly(1,4,4-trifluoro-trans-1-butenylene) polymer), positive values when the value. The coefficients of the helixes had values from -0.168 (poly(1,4,4-trifluoro-trans-1-butenylene)) to 2.268 (polychlorotrifluoroethylene). No significant differences have been observed when the monomers were purely formed by carbon atom (poly(1-methyl-trans-1-butenylene), $(C_5H_8)_{18}$) or by carbon with Cl (poly(1-chloro-trans-1-butenylene), $(C_4H_5Cl)_{18}$). The polymers containing monomers with F and Cl (polychlorotrifluoroethylene, $(CF_2CClF)_n$) had coefficient of the helix with greater values. The poly(1-chloro-trans-1-butenylene), poly(1-methyl-trans-1-butenylene), poly(1,4,4-trifluoro-trans-1-butenylene), polyacrylonitrile, and polychlorotrifluoroethylene show the stability of the helical structures, with a small variation of the helix coefficients when the ended monomers are removed.

Conclusion: Excepting the poly(lactic acid) polymer, all investigated polymers have a real chance to stabilize as helical structures. However, polymers with a higher number of monomers need to be examined to validate the conclusion of this computational study.

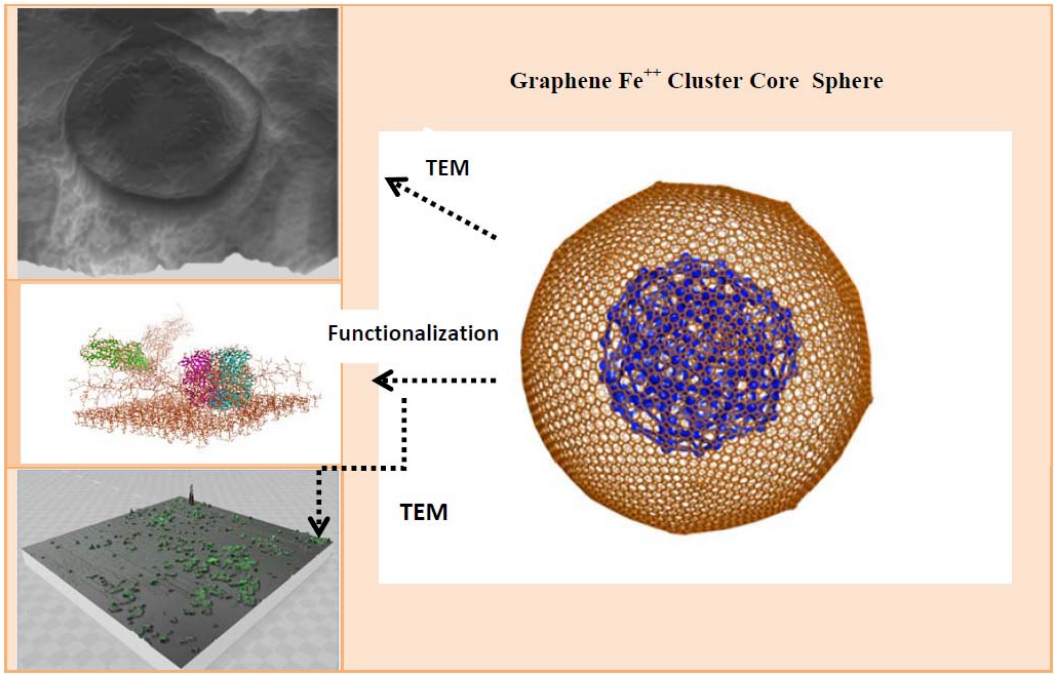


Abstract/Graphical Abstract

MAGNETIC NANOPARTICLE EXPLORED FOR BIOACTIVE MOLECULAR NANODEVICE

Claudiu N. Lungu (1), Michał Bystrzejewski (2), Mircea V. Diudea (1), Ireneusz P. Grudzinskic (3), Magdalena Popławska (4), and Mihai V. Putz (5)

1. Faculty of Chemistry and Chemical Engineering , BabesBolay University, 400028 Cluj, Romania
2. Faculty of Chemistry, University of Warsaw, ul. Pasteura 1, PL-02-093 Warsaw, Poland
3. Faculty of Pharmacy, Medical University of Warsaw, ul. Banacha 1, PL-02-097 Warsaw, Poland
4. Warsaw University of Technology · Faculty of Chemistry, ul. Waryńskiego 1, 00-645 Warsaw, Poland
5. Laboratory of Structural and Computational Physical-Chemistry for Nanosciences and QSAR, Biology-Chemistry Department, Faculty of Chemistry, Biology, Geography, West University of Timisoara, Str. Pestalozzi No. 16, 300115 Timisoara, Romania



NANO-MOD **2018**
16-17 May, Timişoara
West University of Timişoara
*NEW FRONT CHEM 27 (**2018**) 1-36*

Abstract/Graphical Abstract

I HAVE THE GEOMETRY BUT I LOST THE WAY OF ARRIVING TO IT; WHAT I HAVE TO DO?

Lorentz JÄNTSCHI[1,2], Donatella BALINT[2], and Sorana D. BOLBOACĂ[3]

[1] Department of Physics and Chemistry, Technical University of Cluj-Napoca, 400641 Cluj-Napoca, Romania. E-mail: lorentz.jantschi@gmail.com
[2] Chemistry Doctoral School, Babeş-Bolyai University, 400028 Cluj-Napoca, Romania. E-mail: balintdonna@gmail.com
[3] Department of Medical Informatics and Biostatistics, Iuliu Haţieganu University of Medicine and Pharmacy, 400349 Cluj-Napoca, Romania. E-mail: sbolboaca@umfcluj.ro

Background: Three-dimensional quantitative structure-activity relationships (3D-QSAR) are mathematical models able to express the biological activities or properties of compounds as a function of their three-dimensional properties. The quality of the input data in 3D-QSAR analysis is critical since it is related to the quality of the reported model. The objective of our study was to analyze how the quality of the input data, express here as the number of digits of the numerical values, reflects in the model.

Material and method: A dataset of 35 compounds previously discussed by Gramatica et al. [1] relating the toxicity of (benzo)triazoles ((B)TAZs) to the algae *Pseudokirchneriella subcapitata* is used to point out some problems and solutions in 3D-QSAR modeling. The provided *.mol files store the geometric coordinates of the atoms with five decimals. Two procedures were applied to a compound randomly choose from the dataset: optimization with Spartan program at HF 6-31G* level of theory (is the geometry of the compound optimized?) and assessment of how the number of digits in geometry optimization influence the value of descriptors (SMPI - Szeged Matrix Property Indices - family of descriptors was used [2]). Three files were used in the second analysis: the original file (V1), the optimized file (HF 6-31G* theory level) with the full number of digits (10 digits, V2) and respectively with five digits (V3). A weighted difference on the value of the same descriptor calculated on two versions of the molecule was used to quantify the difference.

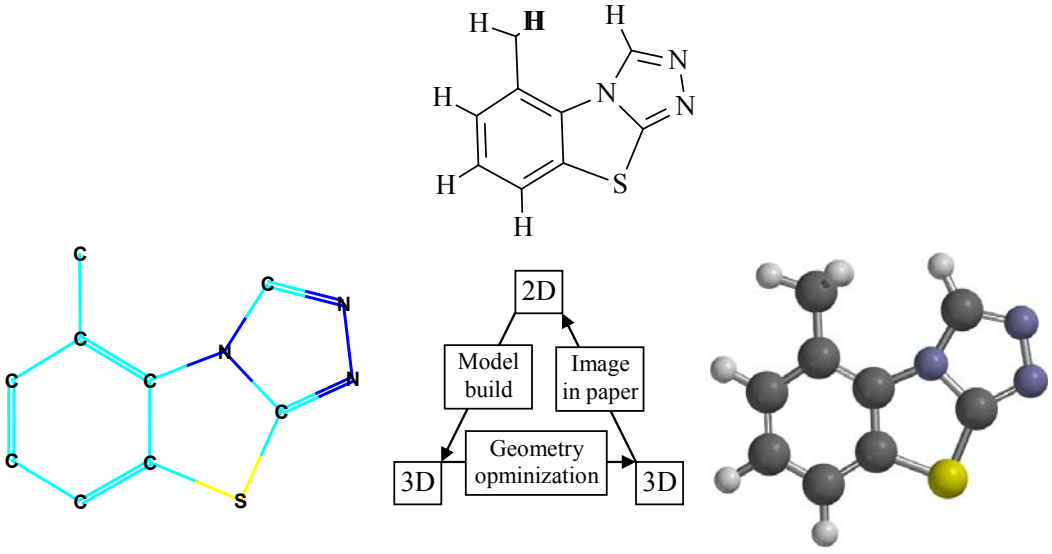
Results: One molecule was randomly chosen to enter in the geometry optimization, and the path obtained (6 steps) show that the geometry was already optimized or very close to the optimum. The number of digits in the file included in the optimization was equal to five, and while the Spartan program works with 10 digits, the optimization was performed. The values of descriptors purely topological were identical for all forms of the input files, while differences have been observed on those descriptors that consider the geometry of the molecule. The average for the whole pool of non-null and non-identical SMPI descriptors was of 1.78% when V1 is compared to V2, and 0.1% when V2 is compared to V3.

Conclusion: The average changes in the value of SMPI descriptors before and after optimization show small changes, showing that the optimization with HF 6-31G* have a minor effect on the calculated properties. The decrease of the number of digits (V2 vs. V3) induces a meaningless change (0.1%) leading to the conclusion that the cutting the number of digits is justified and proofs that the initial geometry was not obtained with HF 6-31G*.

References:

[1] Gramatica P, Cassani S, Roy PP, Kovarich S, Yap CW, Papa E. QSAR Modeling is not "Push a Button and Find a Correlation": A Case Study of Toxicity of (Benzo-)triazoles on Algae. Mol Inform. 2012;31(11-12):817-35. doi: 10.1002/minf.201200075.

[2] Jäntschi L, Bolboacă SD. Szeged Matrix Property Indices as Descriptors to Characterize Fullerenes. Ovidius University Annals of Chemistry 2016;27(2):73-80. doi: 10.1515/auoc-2016-0010



Abstract/Graphical Abstract

NEW APPROACHES CLINICAL STUDIES OF ANTICANCER IN PRE- DRUGS

Bogdan Bumbacila, Constatin Bolcu, Daniel Duda-Seiman, Ana-Maria Putz,Lucian Irimia, & Corina Duda-Seiman

West University of Timişoara, Faculty of Chemistry - Biology Geography, Pestalozzi Str. 16, 300115, Timişoara

Cancer is a group of conditions implying abnormal cell growth in large variety of tissues, cells that possess the ability to invade other tissues (organs). Today there are described more than 100 types of cancer in humans.

Cancer is treated today usually by combining different methods: surgery, pharmacological therapy (cytotoxic chemotherapy), hormonal therapy, targeted therapy (immunotherapy) and radiation therapy. The choice depends on the characteristics of the tumor / cancer like its localization, the characterization of the tumor, the stage of the disease but by far most important it is personalized on the patient and its status.

The great need of therapeutic agents in cancer therapy always led to extensive research in this domain. In the late 20 years, the steps for making a new drug available for therapy always include QSAR studies of the molecules before reaching into preclinical and clinical assessments. These QSAR / QSPR studies usually begin from choosing a series of analogue molecules and describing a Hansch equation for each of the members of the series, taking into account characteristics like the cytotoxic potency but also the potential toxicity because it is known that all the chemical structures that possess anticancer activity are also inducing side effects because of their low specificity on the rapid dividing cell lines.

Combinatorial chemistry today can build libraries of hypothetical molecules which could become real and in silico methods (using software which is characterizing chemical structures by parameters already described in the literature) allow the scientists to predict pharmacological or toxicological characteristics of the substances. So if a molecule could prove useful for therapy further research would be made (synthesis, preclinical and clinical testing) saving important costs and time.

*NEW FRONT CHEM 27 (**2018**) 1-36*

Abstract/Graphical Abstract

MOLECULAR WEIGHT DEPENDENCE OF ADME-TOX PROPERTIES OF CHITIN AND CHITOSAN OLIGOMERS

Madalina Filip, Vasile Ostafe, Adriana Isvoran

Department of Biology-Chemistry and Advanced Environmental Research Laboratories, West University of Timisoara, Romania

Chitin and chitosan are biopolymers having numerous biotechnological and pharmaceutical applications. Using the online servers SwissADME (http://www.swissadme.ch/) and admetSAR (http://lmmd.ecust.edu.cn/admetsar1/predict/), we perform a computational study to reveal the molecular weight dependence of ADME-Tox properties of chitin and chitosan oligomers: bioavailability score, aqueous solubility, skin permeation, substrate/inhibitor of the human cytochromes P450 mainly involved in xenobiotics metabolism, blood brain barrier penetration. Information concerning these properties becomes important as chitin and chitosan oligomers, especially those with six residues or more, reveal some physiological activities, but not all their possible effects were investigated.

Acknowledgment. This work was supported by the grant PN3-P3-285, Polymeric NanoBioMaterials for drug delivery: developing and implementation of safe-by-design concept enabling safe healthcare solutions.

NANO-MOD **2018**
16-17 May, Timișoara
West University of Timișoara
*NEW FRONT CHEM 27 (**2018**) 1-36*

Abstract/Graphical Abstract

DRUG DELIVERY SYSTEMS. STRUCTURE ANALYSIS OF FUNCTIONALIZED SILICA CARRIER AND PRELIMINARY DRUG LOADING - RELEASE TESTS

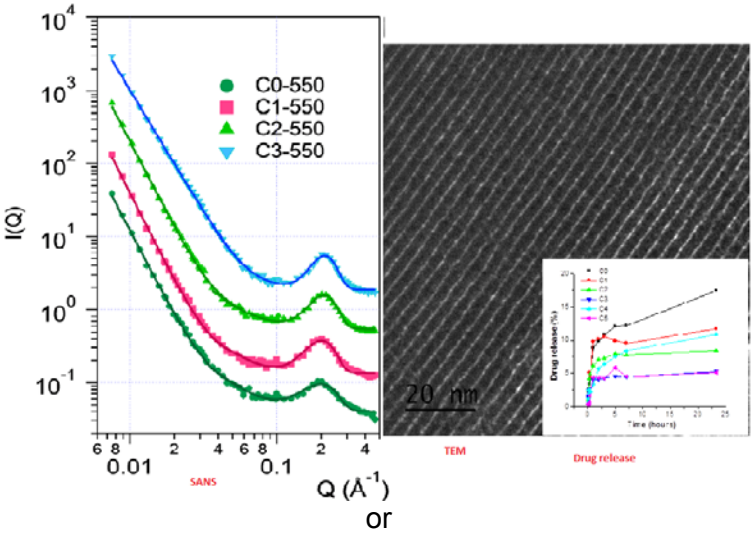
Ana-Maria Putz[1](♣), László Almásy[2], Cătălin Ianăşi[1], Mirela Piciorus[1], Roxana Nicola[1], Adel Len[2], Zoltan Dudas[2], Reka Barabas[3], *Melinda Rigo[3]*, Marius Mirica[4], Bogdan Țăranu[4], Cecilia Savii[1]

[1] Institute of Chemistry Timisoara of Romanian Academy, Timisoara, Romania
[2]Wigner Research Centre for Physics, Budapest, Hungary
[3]Babeș-Bolyai University, Cluj-Napoca, Romania
[4]National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, Romania

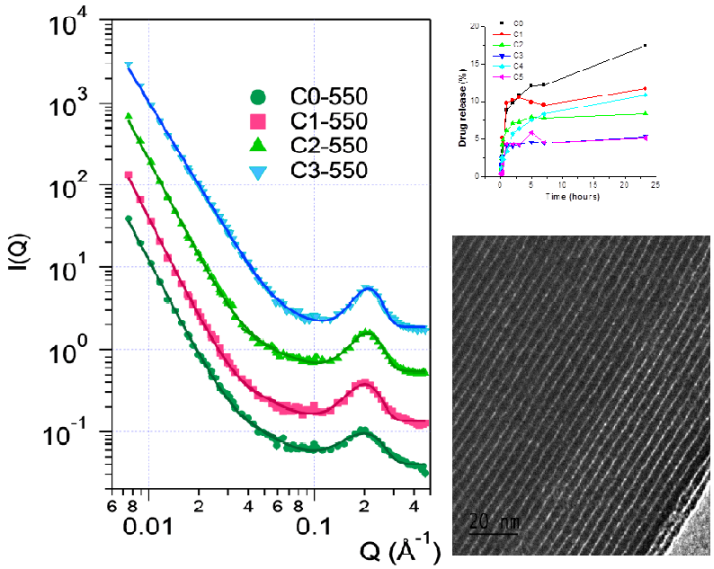
The studies were focused on the relationship between morphology features and synthesis variables, looking for their implications in the drug loading and release capacities. Increasing the amount of methylated tri-alcoxide toward the tetra-alcoxide precursor caused shrinkage of the hexagonally ordered mesoporous structure and also the reduction of the pore diameters, while the total pore volumes and surface areas remain high and suitable for drug loading. In drug release profiles: silica prepared with the largest amount of hydrophobic precursor retained about twice as much of drug, compared with the sample obtained of pure TEOS.

Keywords: drug delivery systems, mesoporous polymeric silica matrices, functionalized precursor

♣ Correspondent author: Tel: +40-256-491818, Fax: +40-256-491824, E-mails: putzanamaria@yahoo.com.


C0-550
C1-550
C2-550
C3-550
I(Q)
Q (Å^{-1})
SANS
20 nm
TEM
Drug release
Time (hours)

or


C0-550
C1-550
C2-550
C3-550
I(Q)
Q (Å^{-1})
Drug release (%)
Time (hours)
20 nm

Abstract/Graphical Abstract

SMOKING AND STRESS – THE NEW OLD ENEMIES

Duda-Seiman D[1], Mancaş S[1], Cosor O[1], Rada M[1], Velimirovici D[1], Tudor S[2], Gligor S[3]

[1]University of Medicine and Pharmacy "Victor Babeş" Timişoara, Dep. of Cardiology, Timişoara, Romania
[2]Policlinica Darimedic, Timis County, Sinandrei, Romania
[3]West University of Timisoara, Fac. of Kinetotherapy and Sport, Timişoara, Romania

There is a very high prevalence of smoking in the world: over 1.1 billion smokers in 2015 [1]. Adult smokers register higher stress levels than non-smokers; age of starting smoking decreased over last years, and stress levels increased in adolescent populations [2].Using validated questionnaires, we will show the correlation between smoking and stress in selected subjects.

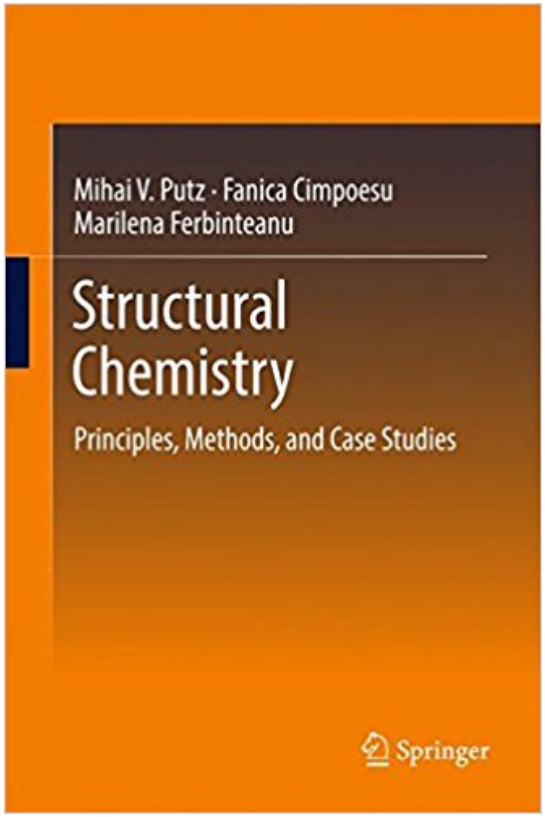
References:
[1] http://www.who.int/gho/tobacco/use/en/, accessed on the 27th of April 2018.
[2] Parrott AC. Does cigarette smoking cause stress? *Am Psychol.* 1999;54(10):817-820.

Abstract/Graphical Abstract

STRUCTURAL CHEMISTRY – PRINCIPLES, METHODS AND CASE STUDIES

Mihai V. Putz (1), Fanica Cimpoesu (2), Marilena Ferbinteanu (3)

1. West University of Timişoara & National Institute of Research and Development for Electrochemistry and Condensed Matter Timişoara (INCEMC)
2. Institute of Physical Chemistry "Ilie Murgulescu", Romanian Academy, Bucharest, Romania
3. Department of Inorganic Chemistry, University of Bucharest, Bucharest Romania



https://www.springer.com/la/book/9783319558738

NANO-MOD **2018**
16-17 May, Timișoara
West University of Timișoara
*NEW FRONT CHEM 27 (**2018**) 1-36*

Abstract/Graphical Abstract

ON THE ELECTRONIC STRUCTURE OF TRIANGULAR POLYAROMATIC HYDROCARBONS WITH SPIN

Ana Maria Toader, Cristina Maria Buta, Fănică Cimpoeșu*

Institute of Physical Chemistry, Splaiul Independentei 202, Bucharest 060021, Romania

In the quest of spintronic based on carbon materials, the academic insight into the bonding of organic molecules with spin plays the role of leading beacon. [1, 2] In this spirit, we present new computational analyses and methodological advances applied on series of polyaromatic systems condensed in the shape of regular triangles. [3] Due to topological reasons, a *n*-triangulene carries *n*-1 unpaired electrons, having groundstates with the *n* spin multiplicity. To be distinguished from the most of previous computational approaches, done by Density Functional Theory (DFT), or Complete Active Space Self Consistent Field (CASSCF) treatments with limited orbital sets, we challenged the problem in the key of Valence Bond (VB) paradigm in both ab initio and phenomenological manners.

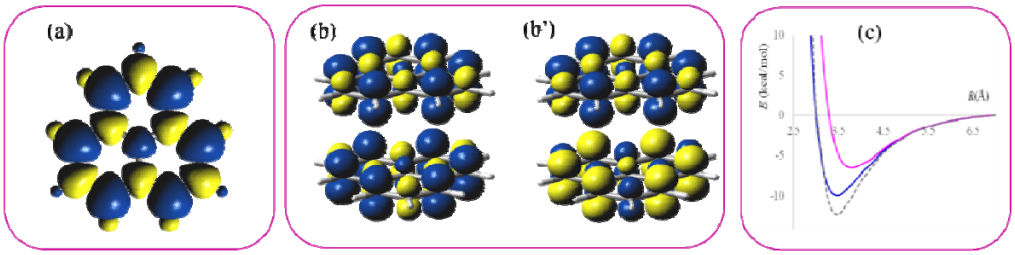


Fig.1 *Results from B3LYP/6-31+G* calculations: (a) the spin density map of phenalenyl radical in groundstate; the phenalenyl dimer at the 3.5 Å inter-planar separation in: (b) High Spin (HS); (b') Broken Symmetry (BS) configurations. (c) the energy curves for phenalenyl dimer as function of interplanar separation obtained by Grimme's D3 correction to B3LYP. The pink curves correspond to HS, the blue lines to BS configuration, while dashed grey lines are singlet profiles emulated from triplet curve and the BS estimation of exchange coupling.*

The Heisenberg spin Hamiltonian was used to simulate the computed spectrum of VB states for the phenalenyl radical (*n*=2), predicting with the fitted parameters the effective VB description of the *n*=3 triangulene and other related systems. The outcome has practical importance in the prospects of spin chemistry on such systems, since the VB ab initio calculations and the CASSCF in the minimal complete π-orbital sets are becoming prohibitive beyond the *n*=2 case. Beyond the technical developments, the results are made transparent to the chemical intuition

exploiting the heuristic language of resonance structures. Moreover, a new clue about the classification of *n*-triangulenes in three equivalency classes is presented. The intermolecular interactions in phenalenyl dimers were analyzed with long-range corrected DFT methods and by VB phenomenological modelling.

References

[1] Dediu, V.A.; Hueso, L.E.; Bergenti, I.; Taliani, C. Spin routes in organic semiconductors. *Nature Materials* **2009**, *8*, 707-716.

[2] Iwamura, H. What role has organic chemistry played in the development of molecule-based magnets?. *Polyhedron* **2013**, *66*, 3–14.

[3] M. Ferbinteanu, C. Buta, A. M. Toader and F. Cimpoesu, *The Spin Coupling in the Polyaromatic Hydrocarbons and Carbon-based Materials*, (pag 327-371) in S. Kaneko, T. Endo, K. Tanaka, D. Hui, P. Mele, T. Tsuchiya, M. Yoshimura, *Carbon-related Materials-in Recognition of Nobel Lectures by Prof. Akira Suzuki in ICCE*

NANO-MOD **2018**
16-17 May, Timișoara
West University of Timișoara
*NEW FRONT CHEM 27 (**2018**) 1-36*

Abstract/Graphical Abstract

STRUCTURAL ANALYSES OF INTERACTING NITROXIDE-BASED ORGANIC RADICALS.

Maria Cristina Buta, Ana Maria Toader, Gabriela Ioniță*

Institute of Physical Chemistry, Splaiul Independentei 202, Bucharest 060021, Romania

This work is a modeling complement developed in the continuation of our extensive investigations devoted to stable organic radicals, [1] used as spin probes in the Electron Paramagnetic Resonance (EPR) measurements of complex supramolecular environments. We use as ancillary tools, state-of-the art methods of quantum chemistry such as Density Functional Theory (DFT) and Valence Bond (VB), as well as phenomenological methods for the spin-spin or spin-field interactions. A thorough analysis is devoted to a series of biradicals containing the TEMPO active group, where TEMPO = (2,2,6,6-tetramethylpiperidin-1-yl)-oxyl. According to our interests in the spin-chemistry, [2] we did a systematic analysis of long-range spin-spin interactions of between nitroxide spin carriers, as function of their mutual placement (distance, bond angles, dihedrals between two N-O groups belonging to different TEMPO moieties. In this view, we worked either with simplified molecular models, or considering the full chemical complexity of certain systems, as suggested in the synopsis outlined in Figure 1.

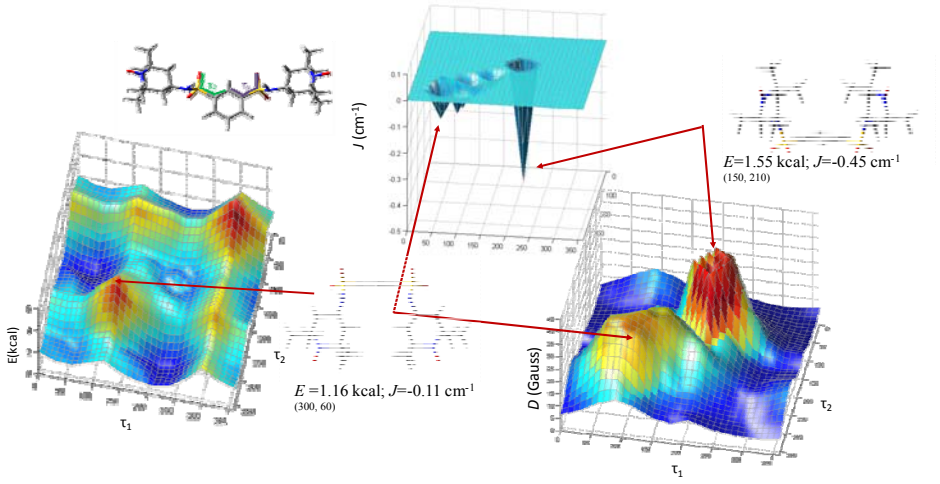


Fig. 1. The mapping of molecular energy (left surface), dipolar interaction (right side) and exchange coupling parameters (top-middle inset), as function of conformational variations in a molecule having two TEMPO moieties attached to a benzene core, via sulfonamide groups.

References

[1] S. Mocanu, I. Matei, S. Ionescu, V. Tecuceanu, G. Marinescu, P. Ionita, D. Culita, A. Leonties and G. Ionita, Complexation of β-cyclodextrin with dual molecular probes bearing fluorescent and paramagnetic moieties linked by short polyether chains, *Phys. Chem. Chem. Phys.*, **2017**, *19*, 27839-27847.

[2] M. Ferbinteanu, C. Buta, A. M. Toader and F. Cimpoesu, *The Spin Coupling in the Polyaromatic Hydrocarbons and Carbon-based Materials*, (pag. 327-371) in S. Kaneko, T. Endo, K. Tanaka, D. Hui, P. Mele, T. Tsuchiya, M. Yoshimura, *Carbon-related Materials-in Recognition of Nobel Lectures by Prof. Akira Suzuki in ICCE*.

NANO-MOD **2018**
16-17 May, Timișoara
West University of Timișoara
*NEW FRONT CHEM 27 (**2018**) 1-36*

Abstract/Graphical Abstract

REVISITING RING STRAIN WITH COMBINED QUANTUM TECHNIQUES

Alice Mischie, Ana Maria Toader, Fanica Cimpoesu*

Institute of Physical Chemistry, Splaiul Independentei 202, Bucharest 060021, Romania

In this work we will revisit several prototypic molecules presenting ring tension, using a series of modern quantum chemical calculation method and post-computational analyses. The molecules with ring strain, because of bond angles enforced out of their usual values, represent a perennial fascination and challenge to the chemical bond theories. The topic is approached in various ways since early accounts being also considered in the light of modern concepts, such as the Bader' s theory of Atoms in Molecules (AIM)[1], and Natural Bond Orbital (NBO) theory[2].

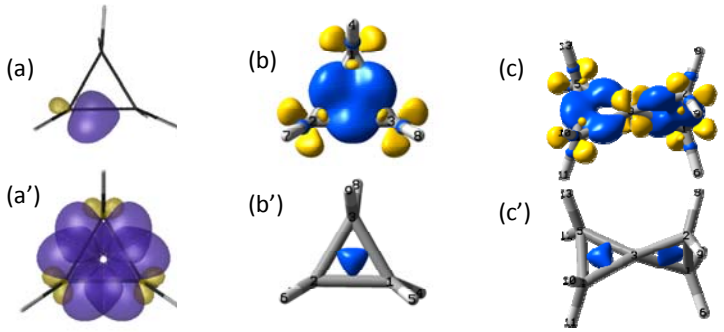


Fig.1 *A synoptic suggestion on performed analyses on ring strain as misdirected valence. (a) a single bonding hybrid as resulted from iterative VB calculations. (a') All the six VB-computed hybrids, involved in bent C-C bonds. (b) the difference density map resulted after extraction of d-type components from the basis set of a B3LYP/cc-pvtz calculation on cyclopropane. (c) the small difference due to the subtraction of f-type primitives from the cc-pvtz basis. (c) and (c'), similar to previous, applied to spiropentane case.*

Using state of the art computation methods, from Density Functional Theory (DFT), to modern versions of Valence Bond (VB) methods, corroborated with revisited ideas of hybridization as quantitative quantum measure[3], we present a series of prototypical molecules, such as the celebrated cyclopropane case and more complex compounds, consisting in several merged tense rings of three or four members. A particular emphasis is done on the issue of basis set components, as carriers of components of the bonding, as suggested in the Figure 1. The density diference maps suggest a relative important role of the d-type components of a basis set, while residual participation of higher terms.

References

[1] Bader, R. "Atoms in Molecules: A Quantum Theory"., Oxford University Press, Oxford, 1994.
[2] Weinhold, F.; Landis, C. "Valency and Bonding. A Natural Bond Orbital Donor-Acceptor Perspective", Cambridge University Press, Cambridge, 2005;
[3] Cimpoesu F, Hirao K, Ferbinteanu M, Fukuda Y, Linert W (2005) New keys for old keywords. case studies within the updated paradigms of the hybridization and aromaticity. Monatsh Chem 136:1071-185

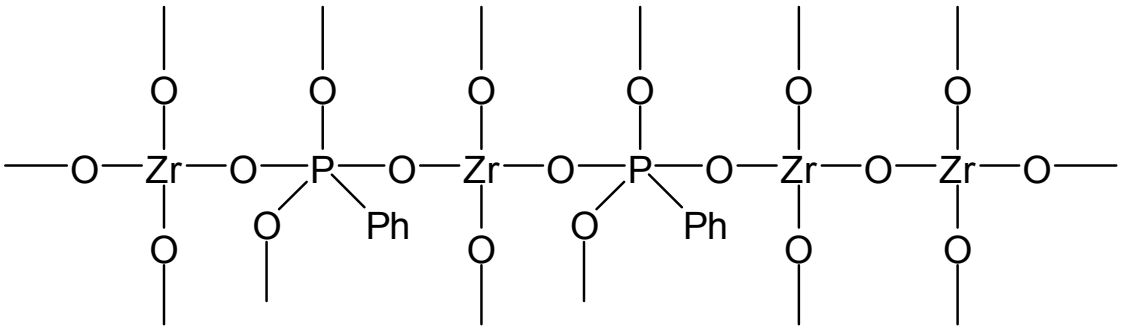
Abstract/Graphical Abstract

ORGANIC-INORGANIC HYBRIDS CONTAINING PHOSPHORUS COMPOUNDS

Vasile Simulescu[1*], **Gheorghe Ilia**[1,2]

[1]Institute of Chemistry Timisoara of Romanian Academy, 24 Mihai Viteazul Blv., 300223 Timisoara, Romania;
[2]West University of Timisoara, Faculty of Chemistry, Biology, Geography, 16 Pestalozzi Street, 300115 Timisoara, Romania;
[*]vsimulescu@gmail.com

In the present work, new organic-inorganic hybrids containing phosphorus compounds were synthesized by using sol-gel method, starting from zirconyl chloride hexa-hydrate ($ZrOCl_2 \cdot 6H_2O$) and phenyl phosphonic acid (PPA) at different molar ratios. All the syntheses were carried out by using water as solvent, at room temperature for 6 hours. After the synthesis was finished, the product was dried for 4 hours at 100°C. These compounds have complex structures and form networks containing Zr-O-Zr and Zr-O-P bonds, as proved by IR and TGA spectra.
Moreover, from IR spectra, no P-O-P, Zr-Zr, P-P or O-O bonds were observed. The connection between zirconium and phosphorus atoms is always made by an oxygen atom. Such organic-inorganic networks are expected to form supramolecular structures and to have applications as catalysts, or in the fields of surface chemistry and supramolecular chemistry.



The structure of the organic-inorganic hybrids containing phosphorus compounds synthesized by sol-gel method

NANO-MOD **2018**
16-17 May, Timișoara
West University of Timișoara
*NEW FRONT CHEM 27 (**2018**) 1-36*

Abstract/Graphical Abstract

QUANTUM ELECTROCHEMICAL SYSTEMS AND MACHINES

Mirela I. Iorga (1,2), Marius C. Mirica (1) and Mihai V. Putz (1,2 *)

1. Laboratory of Renewable Energies-Photovoltaics, R&D National Institute for Electrochemistry and Condensed Matter –INCEMC–Timisoara, Timisoara, Romania
2. Laboratory of Structural and Computational Physical-Chemistry for Nanosciences and QSAR, Biology-Chemistry Department, West University of Timisoara, Timisoara, Romania

Quantum electrochemistry implies concepts, models, and approaches from a wide range of science including mathematics, physics, chemistry, mechanics, engineering, energy, biology, genetics, geology, soil sciences, etc. The rapid development of many areas in nanotechnology has determined the occurrence of new possibilities in the design of functional materials with special properties: optical, photonic, electronic, electrical, thermal, mechanical, chemical, biochemical, and so on [1]. These materials could be realized for specific applications, such as solar cells, rechargeable batteries, biosensors, supercapacitors, and others.

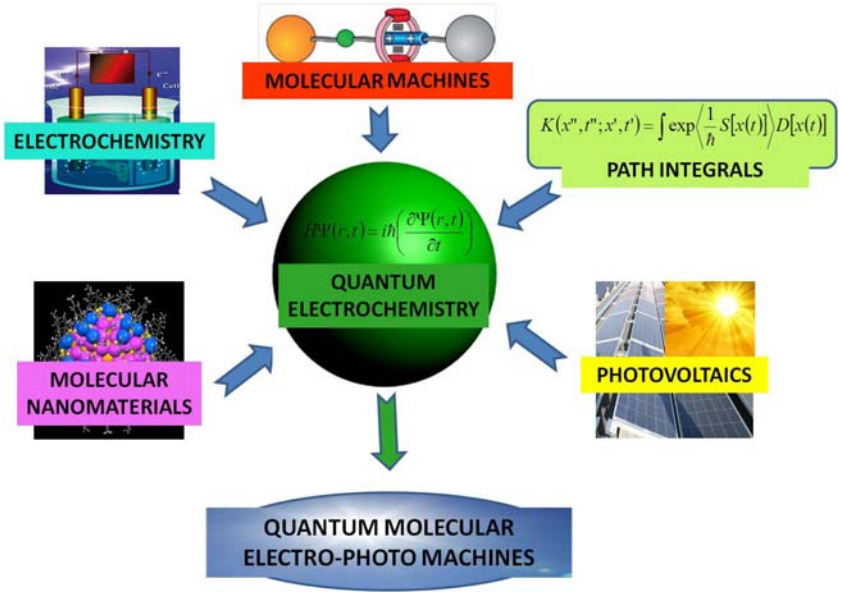


Fig.1. *From micromolecules to molecular dynamic nanosystems*

The route from micromolecules to dynamic molecular nanosystems will be completed using the information obtained from the studies and works carried out so far [2, 3], which will be assembled as shown in Figure 1. Starting from the application of electrochemistry to the specific case of light-activated molecular machines, through the path integral formalism, will be established quantum electrochemical models applicable to molecular machines; these will subsequently be used for various photovoltaic applications, and the final result will be the quantum molecular electro-photo machines.

References

[1] Iorga, M.I; Putz, M.V. Quantum Electrochemistry, in *Explicative Handbook of Nanochemistry*, (Ed.) Putz, M.V., Apple Academic Press, Inc., **2018**.
[2] Iorga, M.; Mirica, M.; Putz, M. Modular Electrochemical Reactivity for Photovoltaics' Machines, in *Nearly Zero Energy Communities*, (Eds.) Visa, I. & Duta, A., Springer Verlag, **2017**, 405-420.
[3] Venturi, M.; Iorga, M.I; Putz, M.V. Molecular Devices and Machines: Hybrid Organic-Inorganic Structures, *Current Organic Chemistry*, **2017**, *21*, 2731-2759.

Acknowledgment. We hereby acknowledge the research project PED123/2017 of UEFISCDI-Romania.

NANO-MOD **2018**
16-17 May, Timișoara
West University of Timișoara
*NEW FRONT CHEM 27 (**2018**) 1-36*

Abstract/Graphical Abstract

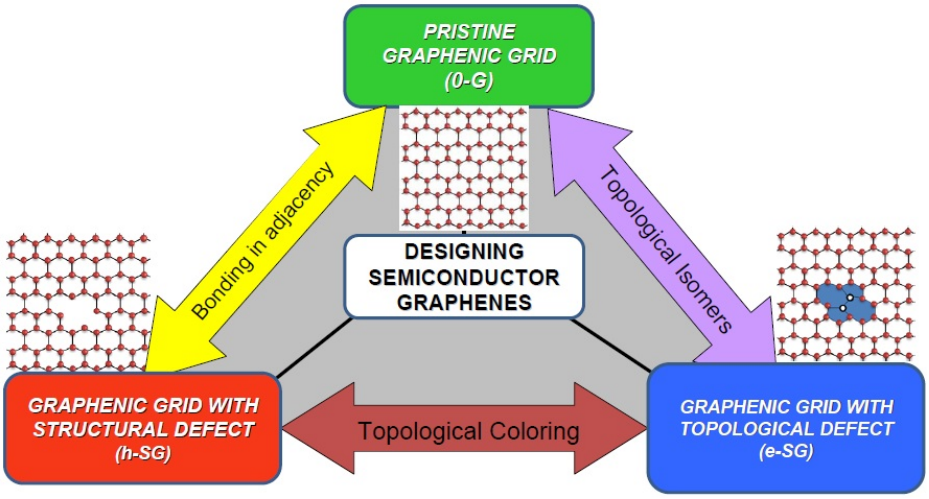
THE PRESENT FUTURE OF THE GRAPHENIC SEMICONDUCTOR

Doru L. Buzatu (1,2), Marius C. Mirica (1) and Mihai V. Putz (1,2 *)

1. Laboratory of Renewable Energies-Photovoltaics, R&D National Institute for Electrochemistry and Condensed Matter –INCEMC–Timisoara, Timisoara, Romania
2. Laboratory of Structural and Computational Physical-Chemistry for Nanosciences and QSAR, Biology-Chemistry Department, West University of Timisoara, Timisoara, Romania;

Graphene, a one-atom-thick honeycomb lattice of carbon atoms has extraordinary optical and electrical features like high electron mobility (100 times greater than silicon). The present challenge is to design and exploit semiconductorgraphene (SG), with controlled conductivity. Accordingly, two new forms of graphene are studied and employed, as new classes of n-doped, and p-doped semiconductors, so producing the so called, e-SG (electron-type semiconductor graphene, based on topological defective Graphene, as appeared by inherent Stone-Wales topological rotations in pristine Graphene 0-G) and h-SG (hole-type semiconductor graphene, when the structurally defective graphene is present).

Keywords: Defective graphenes, Heterojunctions, i/p/n-semiconductors



Acknowledgment. We hereby acknowledge the research project PED123/2017 of UEFISCDI-Romania.

NANO-MOD **2018**
16-17 May, Timișoara
West University of Timișoara
*NEW FRONT CHEM 27 (**2018**) 1-36*

Abstract/Graphical Abstract

CORRELATION OF CHEMICAL BONDS ORDERS CALCULATED BY MOLECULAR ORBITALS METHOD WITH SOME PROPERTIES OF SIMPLE AND COMPLEX SUBSTANCES

Daniela DASCĂLU [1,2,♣], Beatrice VLAD-OROS [1,2], Delia ISAC [1,2], Adriana ISVORAN [1,2]

[1]West University of Timisoara, Faculty of Chemistry, Biology, Geography, Department of Biology-Chemistry, 16 Pestalozzi, Timisoara, Romania; [2]Advanced Environmental Research Laboratories, 4 Oituz, Timisoara, Romania
[♣]e-mail: daniela.dascalu@e-uvt.ro

A bound polyatomic system has a real existence if the bond order is positive, regardless its value. Its correlations are made with the bonds length of the inorganic and organic substances [1, 2]. The bond orders between two atoms of a molecule or molecular ion were calculated as half of the difference between the number of electrons (n) of bonding MO and the number of electrons (n*) of antibonding MO [3a]. For the 13 molecular species (diatomic molecules, derivative molecular cations and anions) of the elements from first two periods correlations were made between their electronic configurations, calculated bond orders and diamagnetic and paramagnetic character [4a]. The strength of corresponding homonuclear bonds and the stability of those compounds can be explained and also correlated with internuclear distances from the literature data [4b]. The calculations for electric moments (μ) of dipoles and for contribution coefficients (c_A, c_B) of wave functions (ψ_A, ψ_B) to the wave functions σ bonding MO and σ* antibonding MO were made by choosing 10 heteronuclear bonds [3a]. The bond orders of the 14 metals from 4th period analysed in this paper were calculated by dividing the number of electrons pairs of the n metal atoms each contains to the number of bonding MO of the system. The obtained results can underlie the interpretation of physical and mechanical properties [3b]. As applications, for the organic compounds with polycentric π bonds, diazonium salts of p-aniline, p-dimethylaminoaniline and 2-naftilamine were selected. The calculations were made only for the π electrons systems of the molecules (π approximation) and the bond orders (p_{qp} sau π_{qp}) meet the Hückel molecular orbitals method (HMO) requirements [5, 6]. It was proved that the structural and energetic indices calculated by HMO method, using Streitwieser parameters [7] confirm the acidic, oxidant and electrophilic character of analysed diazonium cations.The motivation of choosing these systems is related to the uses of the studied substances.

REFERENCES

1. Coulson, C.A.,The electronic structure of some polyenes and aromatic molecules. VII Bonds of fractional order by molecular orbital method, *Proc. Roy. Soc. (London) A*, **1939**, *169*, 413-428.
2. Coulson, C.A., Longuet-Higgins, H.C. Developpements recent de la theorie de la reactivite des molecules possedant des doubles liaisons conjuguees, *Rev. Sci.*, **1947**, ***85***, 929-938.
3. Chiriac, V., Chiriac, V., Dascălu, D., Isac, D. *Curs de chimie generală*, Ed. Mirton, Timişoara, 2003; a) pp. 78-84, b) pp. 102-105.
4. Marcu, G., Brezeanu, M., Bâtcă, A., Bejan, C., Cătuneanu, R. *Chimie anorganică*, Ed. Didactică şi pedagogică, Bucureşti, 1984; a) pp. 168-170, b) pp. 105-114.
5. Mulliken, R.R. A new electroaffinity scale together with the data on valence states and on valence ionization potentials and electron affinities, *J. Chem. Phys.*, **1934**, *2*, 782-793.
6. Lennard-Jones, J.E. Electronic structure of some polyenes and aromatic molecules, Proc. Roy. Soc. (London) A., 1937, **158**, 280-296.
7. Streitwieser, A. jr. *Molecular Orbital Theory for Organic Chemists*, John Wiley, New York, 1961.

NANO-MOD **2018**
16-17 May, Timişoara
West University of Timişoara
*NEW FRONT CHEM 27 (**2018**) 1-36*

Abstract/Graphical Abstract

SYNTHESIS AND CHARACTERIZATION OF IRON OXIDE NANOPARTICLES COATED WITH MESOPOROUS SILICA VIA SURFACTANT TEMPLATE SOL-GEL METHOD. INFLUENCE OF CTAB/SiO_2 RATIO UPON MORPHO-TEXTURAL PROPERTIES*

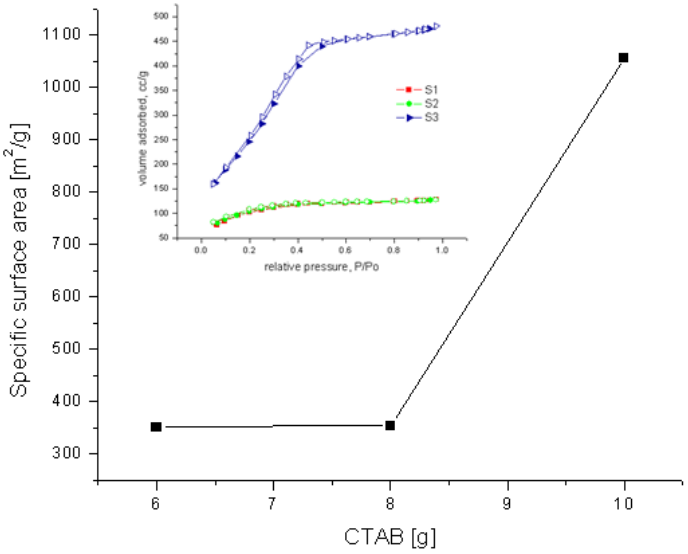
Roxana Nicola[(1♣)], **Otilia Costişor**[(1)], **Cătălin Ianăşi**[(1)], **Radu Lazău**[(2)], **Liviu Săcărescu**[(3)], **Daniel Nižňanský**[(4)], ***Cecilia Savii***[(1)]

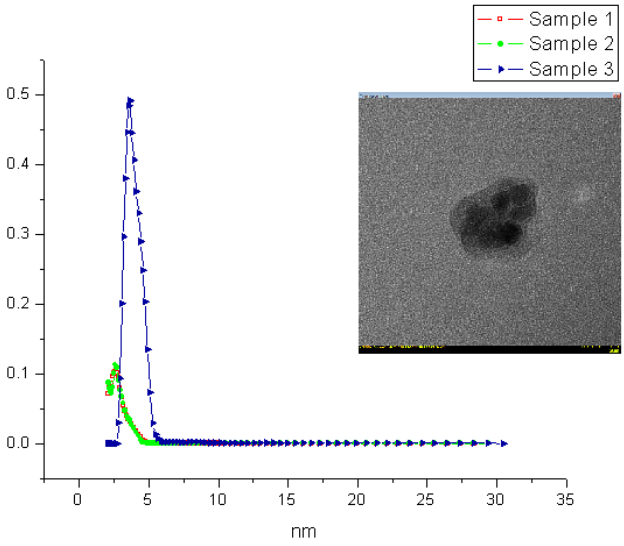
[1]Institute of Chemistry Timişoara of Romanian Academy, 24 Mihai Viteazul Bd., 300223, Timişoara, România
[2]"Politehnica" University of Timişoara, Faculty of Industrial Chemistry and Environmental Engineering, Vasile Pârvan Bd., No. 6, 300223, Timişoara, România
[3]Institute of Macromolecular Chemistry "Petru Poni", Grigore Ghica Voda Alley, No. 41A, 700487, Iaşi, România
[4]Charles University in Prague, Faculty of Science, Albertov 6, 128 43, Praque, Czech Republic

Synthetic research related to iron oxide/mesoporous silica nanocomposites has focused on the tuning of the material`s properties, such as, the silica shell thickness, pore size and total pore volumes. In this concern, in the paper, we studied the influence of CTAB/SiO_2 molar ratio. At first, the iron oxide particles were synthesized by co-precipitation method. Than the resulted iron oxide nanoparticles where coated with silica using cethyl-trimethyl ammonium bromide (CTAB) as template. The coated and uncoated iron oxide samples were submitted to a comparative study. The influence of CTAB/SiO_2 molar ratio upon the mentioned properties of the silica shell was obvious.

Keywords: iron oxide, mesoporous silica, sol-gel, CTAB, nanocomposites.

♣ Correspondent author: Tel:+40-256-491818; Fax: +40-256-491824; cc.roxana@yahoo.com.


Specific surface area [m²/g]
CTAB [g]
volume adsorbed, cc/g
relative pressure, P/Po
S1
S2
S3


Sample 1
Sample 2
Sample 3
nm

Abstract/Graphical Abstract

TEMPLATE FREE SPHERICAL SILICA SOL-GEL SYNTHESIS. ROLE OF PRECURSOR CONCENTRATION IN STOEBER PROCESS

Mirela PICIORUŞ[1], Cătălin IANĂŞI[1], Ana-Maria PUTZ[1], Paula SFIRLOAGA[2], Cecilia SAVII[1]

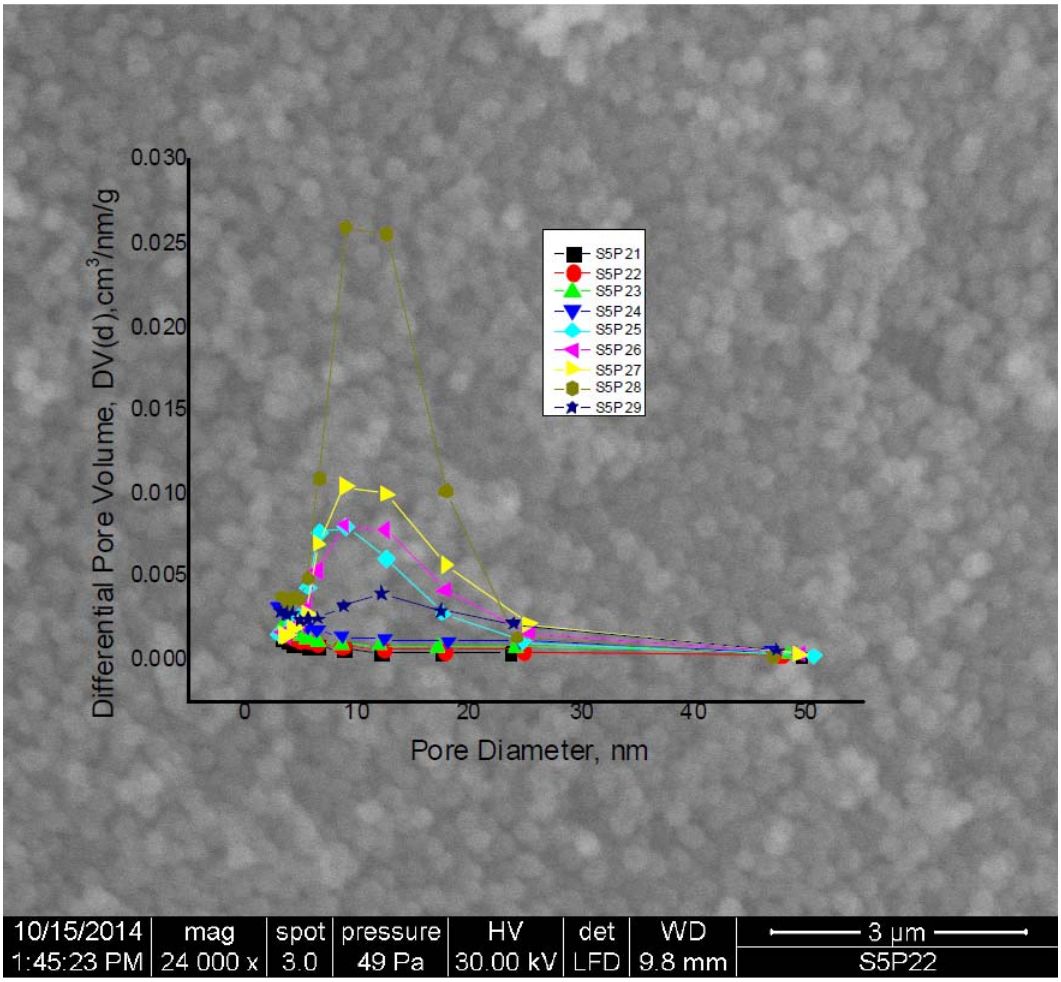
[1]Institute of Chemistry Timisoara of the Romanian Academy, 24 Mihai Viteazu Bdl.,300223, Timisoara, Romania

[2]National Institute for Research and Development in Electrochemistry and Condensed Matter, 144 Prof. dr. Aurel Paunescu Podeanu Str., Timisoara, Romania

Correspondent author: Tel: +40-256-491818, Fax: +40-256-491824, E-mails: mirela_taerel82@yahoo.com

Spherical silica nanoparticles were synthesized by sol-gel process from tetra-ethyl-orthosilicate without using template. The TEOS: H_2O: ETOH: NH_3 mole ratio was n: 0.43: 0.789: 0.06, where n varied in the 0.022÷ 0.31 range. SEM images showed that almost spherical in shape silica nanoparticles were obtained. The synthesized particles have the diameter between 3 and 9 nm and variable surface area, specifically between 13 and 112 m^2/g. Pore size distribution was significantly narrower for samples with the higher precursor concentration. The particles size decreases gradually as the concentration of the TEOS increases. The obtained results showed the precursor concentration effects.

Keywords: Stoeber, narrower, precursor


Differential Pore Volume, DV(d),cm3/nm/g
0.030
0.025
0.020
0.015
0.010
0.005
0.000
0
10
20
30
40
50
Pore Diameter, nm
S5P21
S5P22
S5P23
S5P24
S5P25
S5P26
S5P27
S5P28
S5P29
10/15/2014
1:45:23 PM
mag
24 000 x
spot
3.0
pressure
49 Pa
HV
30.00 kV
det
LFD
WD
9.8 mm
3 µm
S5P22

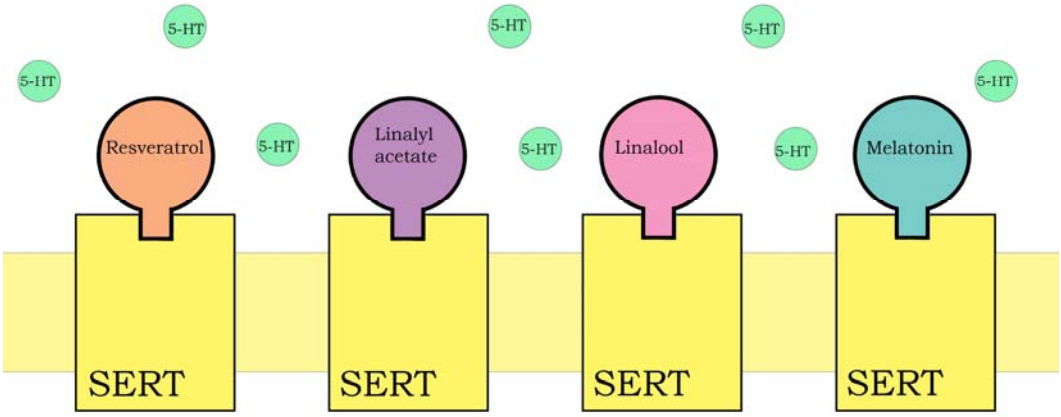
Abstract/Graphical Abstract

MELATONIN, RESVERATROL, LINALOOL AND LINALYL ACETATE-NEW PERSPECTIVES IN TREATMENT OF DEPRESSION.

Ana-Maria Udrea, Alin Puia, Iulia Alexandrescu and Speranta Avram

University of Bucharest, Faculty of Biology, Department of Anatomy, Animal Physiology and Biophysics, Bucharest, Romania

Antidepressants and antipsychotics drugs represent the most commonly prescribed drugs used for the treatment of neuropsychiatric disorders. Their effectiveness and adverse effects are still the subject of many studies. Natural compounds, with reduced side effects but still unknown molecular mechanisms at brain membrane receptors, represent an innovative opportunity for management of neuropsychiatric disorders in pregnancy and a critical scientific target. Here, we have predicted using computational 2D-QSAR (Quantitative Structure-Activity Relationship) and 3D-QSAR methods: (i) the binding affinities of natural compounds, namely melatonin, resveratrol, linalool and linalyl at serotonin transporter (SERT), deeply involved in neuropsychiatric disorders mechanisms and (ii) their transfer index through placenta. Our results showed that natural compounds present similar biological activity on Serotonin Transporter with medication used in treatment of depression.



Abstract/Graphical Abstract

PREDICTION OF ADME-TOX PROPERTIES OF POLYLACTIC ACID OLIGOMERS

Diana Larisa Roman, Marin Roman, Silvana Ceauranu, Vasile Ostafe, Adriana Isvoran

Department of Biology-Chemistry and Advanced Environmental Research Laboratories, West University of Timisoara, Romania

Within this study we reveal the ADME-Tox properties and pharmacokinetics of polylactic acid oligomers: aqueous solubility, skin permeation, blood brain barrier permeation, substrate/inhibitor of the human cytochromes P450 mainly involved in xenobiotics metabolism, carcinogenicity, mutagenicity. Information concerning these properties becomes important as these oligomers have numerous applications in medical and pharmaceutical industries.

Acknowledgment. This work was supported by the grant PN3-P3-285, Polymeric NanoBioMaterials for drug delivery: developing and implementation of safe-by-design concept enabling safe healthcare solutions.

NEW FRONTIERS IN CHEMISTRY:

PROCEEDING OF ABSTRACTS

Green nanochemistry - application of the safe by design principle for obtaining new nanomaterials

7 June 2018, Timişoara

Editors:

ADRIANA ISVORAN
VASILE OSTAFE
West University of Timişoara
Faculty of Chemistry, Biology, Geography
Biology-Chemistry Department
Timişoara, ROMANIA

WEST UNIVERSITY OF TIMISOARA
ADVANCED ENVIRONMENTAL RESEARCH LABORATORIES
&
SOCIETATEA ROMÂNĂ DE BIOCHIMIE ȘI BIOLOGIE MOLECULARĂ, FILIALA BANAT

PN3–P3-284/2017 NanoBioMateriale polimerice pentru eliberarea de medicamente: dezvoltarea și implementarea conceptului de safe-by-design care să permită soluții de asistență medicală în condiții de siguranță/ Polymeric NanoBioMaterials for drug delivery: developing and implementation of safe-by-safe-design concept enabling safe healthcare solutions

www.uvt.ro http://www.elearning-chemistry.ro/lcam1/home-2/wut-uvt/ http://www.srbbm-banat.ro/

WORKSHOP

Green nanochemistry - application of the *safe by design* principle for obtaining new nanomaterials

07.06.2018

Program

12.00 12.10	Prof. Dr. Vasile OSTAFE Opening word – project presentation
12.10 12.15	Conf. Dr. Cătălina Ancuța Opening speech from the leadership of the Faculty of Chemistry, Biology, Geography
	Session 1 Chairman Prof. Dr. Mihai Putz
12.15 12.45	Prof. Dr. Vasile OSTAFE *Safe by design* principle
12.45 13.15	Prof. Dr. Adriana Isvoran, A computational approach of the concept of *safe by design*. Application for chitin and chitosan oligomers
13.15-13.30	Drd. Gheorghița Menghiu, The exposure effect of organisms to

	nanoparticles and nanomaterials: genetic and epigenetic modifications.
13.30-13.45	**Break** **Session 2** **Chairman Prof. dr. Vasile Ostafe**
13.45-14.00	**Drd. Bianca Boroș Ecotoxicity of nanomaterials in the aquatic and terrestrial environments**
14.00-14.15	**Drd. Marin Roman, Computational assessment of ADME-Tox profiles of some polylactic acid oligomers**
14.15-14.30	**Drd. Bianca Vulpe, Ecotoxicology test at enzymatic level. Chromatography and spectrophotometer analysis for invertase, sulphatase and acid phosphatase.**
14.30-14.45	**Asist. Dr. Diana Larisa Roman, Safety assessment of poly(3-hydroxybutyrate) small oligomers**
14.45-15.00	**Drd. Adina Matica, Environmental impact of nanoparticles: effect on soil and water microorganisms**
15.00-15.15	**Prof. Dr. Mihai Putz, Orthogonal photochemistry-electrochemistry with molecular machines**
15.15 **15.30**	**Alexandru Pahomi, Preparation and characterization of nano chitosan**
15.30	**Prof. Dr. Vasile Ostafe** **Concluding remarks**

SAFE BY DESIGN PRINCIPLE

***Vasile Ostafe*[(1,2)] ♣**

[1]Department of Biology-Chemistry, Faculty of Chemistry, Biology, Geography, West University of Timisoara

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

ABSTRACT

Nanotechnology although has contributed to the development of new products with new functions, raise new safety issues. Nanoparticles of a material usually have very different qualities from those that the material has at its ordinary scale and some of these new properties may affect the quality of the environment and the human health. The concerns are rationalized due to our previous experience with health risks caused by the release into the nature of other ultrafine particles such as asbestos and air pollution with dust (PM 2.5). To avoid such incidents, the idea to analyze the safety issues in both the R&D and design phases of preparation of a new product was embedded in the concept safe-by-design (SbD). This concept targets to reduce the overall environmental and human health risks at an early phase of the innovation process, creating an integrated research strategy. In this way the functionality of a new product will be correlated with the harmfulness and safety issues generated by that product. SbD will deal with safety measures for the prevention of accidents, illnesses, or environmental damage at any stage of production of a material, from it design until its end-of-life. SbD used the doctrine of „fail early, fail often", which means doing many safety tests *in vitro* and *in silico* to learn about issues and interactions that could decrease safety. In close relation with SbD concept is the notion of „responsibility for safety", linked to concept of „responsible research and innovation".

Keywords: safe by design, nanotechnology, safety issues, responsibility for safety

Acknowledgements –This work was supported by the grant PN3-P3-285, Polymeric NanoBioMaterials for drug delivery: developing and implementation of safe-by-design concept enabling safe healthcare solutions.

♣ Correspondent author: E-mail: vasile.ostafe@e-uvt.ro; Tel. 0040755240153

GREEN-NANOCHEM **2018**
7 June, Timişoara
West University of Timişoara
*NEW FRONT CHEM 27 (**2018**) 37-49*

A COMPUTATIONAL APPROACH OF THE CONCEPT OF SAFE BY DESIGN. APPLICATION FOR CHITIN AND CHITOSAN OLIGOMERS

***Mădălina Filip*[(1,2)], *Miruna Gug*[(1,2)], *Vasile Ostafe*[(1,2)], *Adriana Isvoran*[(1,2)]♣**

[1]Department of Biology-Chemistry, Faculty of Chemistry, Biology, Geography, West University of Timisoara
[2]Advanced Environmental Research Laboratories, West University of Timisoara

ABSTRACT

The concept of safe by design can be addressed using computational studies. The bases of computational approaches concerning the design of safe biomaterials are explained within this study. Furthermore, these approaches are applied for predicting the pharmacokinetics properties and toxicological endpoints of chitin and chitosan oligomers.

Keywords: safe by design, computational approach, chitin oligomers, chitosan oligomers.

Acknowledgements –This work was supported by the grant PN3-P3-285, Polymeric NanoBioMaterials for drug delivery: developing and implementation of safe-by-design concept enabling safe healthcare solutions.

♣ Correspondent author: Tel:+40256592634, Fax: :+40256592634, E-mail: adriana.isvoran@e-uvt.ro

GREEN-NANOCHEM **2018**
7 June, Timişoara
West University of Timişoara
*NEW FRONT CHEM 27 (**2018**) 37-49*

THE EXPOSURE EFFECT OF ORGANISMS TO NANOPARTICLES AND NANOMATERIALS: GENETIC AND EPIGENETIC MODIFICATIONS

Gheorghita MENGHIU [(1,2)], ***Vasile OSTAFE*** [(1,2♣)]

[1] Advanced Environmental Research Laboratories, Oituz 4, Timisoara 300086, Romania
[2] West University of Timisoara, Faculty of Chemistry, Biology, Geography, Pestalozzi 16, Timisoara 300115, Romania

ABSTRACT

The exposure of organisms to nanoparticles and nanomaterials is increasingly used, but their effect on DNA or RNA sequences and genes function is not fully known. Recent studies show that in mammalian cells exposed to different nanoparticles as gold, silver, titanium dioxide, cerium oxide, silica, cobalt, chromium or carbon nanotubes, the DNA undergoes damaging and proteins expression is strongly influenced. Changes in DNA methylation, in DNA repair pathways or post-translational modifications of histones and noncoding RNA, were also identified. Nanomaterials obtained from chitosan, polylactic acid, poly (lactic-co-glycolic acid) or polyhydroxyalkanoate are also widely investigated for drug delivery and tissue engineering applications, but their genotoxic potential is also a challenge at cellular level.

Keywords: nanoparticles, nanomaterials, epigenetic modifications, DNA, RNA

Acknowledgements
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.

♣ Correspondent author: Tel:, Fax:, E-mails:

GREEN-NANOCHEM **2018**
7 June, Timişoara
West University of Timişoara
*NEW FRONT CHEM 27 (**2018**) 37-49*

ECOTOXICITY OF NANOMATERIALS IN THE AQUATIC AND TERRESTRIAL ENVIRONMENTS

BOROS Bianca-Vanesa [(1)] ♣, ***OSTAFE Vasile*** [(1)]

[1] Department of Biology-Chemistry, West University of Timisoara, Pestalozzi 16, Timisoara, Romania & Advanced Environmental Research Laboratories, West University of Timisoara, Oituz 4, Timisoara, Romania

ABSTRACT

The development of NMs used in medicine exhibits an exponential growth, thus the safety of NMs is of high priority and important amounts of these materials could have been introduced into the environment. Thus, the investigation of NMs' ecotoxicity in the environment is of high interest.
Ecotoxicity measurements of NMs are conducted on different trophic levels including plants, invertebrates, and vertebrates. Ecotoxicity assays have been standardized for soluble substances, and thus, their adaptation for NMs is needed.
In this presentation, the ecotoxicity of NMs is described in comparison with their base substances in both aquatic and terrestrial ecosystems.

Keywords: ecotoxicity assays, adaptation of assays for nanomaterials, aquatic and terrestrial assays guidelines, comparison of ecotoxicity of nanomaterials and their base substances

This work is supported by Grant ID: 14/2017 PN3-P3-285, GoNanoBioMat - Polymeric nanobiomaterials for drug delivery: developing and implementation of safe-by-design concept enabling safe healthcare solutions.

♣ Correspondent author: Tel: 0741 011 264, E-mails: bianca_boros2006@yahoo.com; bianca.boros91@e-uvt.ro

GREEN-NANOCHEM **2018**
7 June, Timişoara
West University of Timişoara
*NEW FRONT CHEM 27 (**2018**) 37-49*

COMPUTATIONAL ASSESSMENT OF ADME-TOX PROFILES OF SOME POLYLACTIC ACID OLIGOMERS

***Marin Roman*, *Diana Larisa Roman*, *Silvana Ceauranu*, *Vasile Ostafe*, *Adriana Isvoran*[♣]**
Department of Biology-Chemistry and Advanced Environmental Research Laboratories, West University of Timisoara, Romania

ABSTRACT

Polylactic acid (PLA) is a compound widely used in human medicine especially for tissue engineering and drug delivery systems and in cosmetics for correction of scars and wrinkles. There are a few known side effects of PLA on humans, such as allergic reaction, angioedema, hypersensitivity reactions. In the human body, PLA is degraded to its oligomers that are metabolized and their effects are not known. In this study we have used Swiss Target Prediction, admetSAR, Toxtree and EndocrineDisruptome computational tools for predicting the molecular targets and respectively for assessing the ADME-Tox profiles and pharmacokinetic properties of small oligomers of polylactic acid.

Keywords: polylactic acid, ADME-Tox properties, pharmacokinetics.

Acknowledgements – This work was supported by the grant PN3-P3-285, Polymeric NanoBioMaterials for drug delivery: developing and implementation of safe-by-design concept enabling safe healthcare solutions.

♣ Correspondent author: Tel. +40745901850:, Fax:+40256592620, E-mail: adriana.isvoran@e-uvt.ro

GREEN-NANOCHEM **2018**
7 June, Timişoara
West University of Timişoara
*NEW FRONT CHEM 27 (**2018**) 37-49*

ECOTOXICOLOGY TEST AT ENZYMATIC LEVEL. CHROMATOGRAPHY AND SPECTROPHOTOMETER ANALYSIS FOR INVERTASE, SULPHATASE AND ACID PHOSPHATASE

Bianca Vulpe [1,2], Monica Gusa [2], Silviu Cotreanți [2],Andra Pandele[2], Vasile Ostafe [1,2]

[1]Advanced Research Environmental Laboratories, Multidisciplinary Research Platform "Nicholas Georgescu - Roegen", 4 Street Oituz, Timisoara 300086, Romania

[2]Department of Biology – Chemistry, Faculty of Chemistry – Biology – Geography, West University of Timisoara, 16 Street Pestalozzi, Timisoara 300115, Romania

ABSTRACT

This study aims to create a ecotoxicological battery tests by selecting important enzymes from major metabolic pathways or tissue. One enzyme present one reaction rate in optimal conditions to function. Our study wants to test whether nanocompounds can influence enzyme activity to reduce macromolecular tests. To test the activity of enzymes, we used chromatographic analyses and spectrophotometer analyses. Until now we used acid phosphatase, sulphatase and invertase and we optimize the method for each enzymes. The result show us that concentration of buffer and the pH influence the results and we tried to optimized the method for a good results.

Keywords: enzymes, ecotoxicologiacal battery test, invertase, acid phosphatase,sulphatase

GREEN-NANOCHEM **2018**
7 June, Timişoara
West University of Timişoara
*NEW FRONT CHEM 27 (**2018**) 37-49*

SAFETY ASSESSMENT OF POLY (3-HYDROXYBUTYRATE) SMALL OLIGOMERS

***Diana Larisa Roman*, *Marin Roman, Silvana Ceauranu, Vasile Ostafe, Adriana Isvoran*♣**
Department of Biology-Chemistry and Advanced Environmental Research Laboratories, West University of Timisoara, Romania

ABSTRACT

Polyhydroxybutyrate acid (PHB) is the most commonly occurring polyhydroxyalkanoate (PHA) revealing biodegradability, biocompatibility and a broad spectrum of physical properties. These characteristics conduct to diverse applications of PHB in medicine and pharmacy. To the best of our knowledge, there is not information concerning the safety profile of PHB oligomers. In this study we have used Swiss Target Prediction, admetSAR, Toxtree, EndocrineDisruptome and PASS computational tools for assessing the safety profiles and the toxicological endpoints of small oligomers of polyhydroxybutyrate acid (2 to 16 monomers). These oligomers are predicted to not reflect cardiotoxicity and mutagenicity. They emphasize a low probability to interact with the human androgenic receptor, a low carcinogenic potential and medium values for the skin penetration coefficients. There are a few predicted side effects of PHB on humans: respiratory toxicity and eyes irritation.

Keywords: polyhydroxybutyrate acid, safety profile, toxicological endpoits

Acknowledgements – This work was supported by the grant PN3-P3-285, Polymeric NanoBioMaterials for drug delivery: developing and implementation of safe-by-design concept enabling safe healthcare solutions.

♣ Correspondent author: Tel. +40745901850:, Fax:+40256592620, E-mail: adriana.isvoran@e-uvt.ro

GREEN-NANOCHEM **2018**
7 June, Timişoara
West University of Timişoara
*NEW FRONT CHEM 27 (**2018**) 37-49*

ENVIRONMENTAL IMPACT OF NANOPARTICLES: EFFECT ON SOIL AND WATER MICROORGANISMS†

MATICA Adina, [1,2] ***OSTAFE Vasile***[1,2]♣

[1,2] West University of Timisoara, Department of Biology – Chemistry (Pestalozzi 16, Timisoara, 300315) & Advanced Environmental Research Laboratories (Oituz 4, Timisoara 300086, Romania)

ABSTRACT

Nanotechnology is one of the most researched scientifical fields, with over 1300 commercial products that have various applications in medical fields, fuel additives, textile and cosmetics industry, plastics and others. While being very useful, there is still insufficient information about how engineered nanoparticles can affect the environment. Since these advanced materials are much smaller than traditional ones, they possess unique chemical properties, high reactivity, and low solubility, the impact towards soil and water ecosystems is even more difficult to assess. Standardized test protocols for soluble chemicals may not be suitable for testing nanomaterials, thus scientists are working on developing new procedures to evaluate the impact of nanoparticles on water and soil ecosystems, especially key organisms.

Keywords: nanotechnology, nanoparticles, toxicity, biodegradability

Acknowledgements

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

♣ Correspondent author: +40-755240153, vasile.ostafe@e-uvt.ro

GREEN-NANOCHEM **2018**
7 June, Timişoara
West University of Timişoara
*NEW FRONT CHEM 27 (**2018**) 37-49*

ORTHOGONAL PHOTOCHEMISTRY-ELECTROCHEMISTRY WITH MOLECULAR MACHINES

Mihai V. Putz (1,2, *), Mirela I. Iorga (1,2), and Corina Seiman (1)

1. Laboratory of Structural and Computational Physical-Chemistry for Nanosciences and QSAR, Biology-Chemistry Department, West University of Timisoara, Timisoara, Romania;
2. Laboratory of Renewable Energies-Photovoltaics, R&D National Institute for Electrochemistry and Condensed Matter –INCEMC– Timisoara, Timisoara, Romania

ABSTRACT

In the context of green-organic physical-chemistry application the recent 2016 Nobel awarded as "the smallest built machines in the world" – the molecular machines are employed in an coupled photo-electro-chemical ("orthogonal") transformations towards acquiring the closing cycle by which the photo-activated molecules become electronically activated and carriers which can be switched back through passing an electrochemical bath thereof; the mechanism for the total difference in Gibbs energy is proposed by means of coupling path integrals of partition functions by specific types of physical-chemical transformations undergone, while the molecular machines relationship with the perpetual mobile machines are also discussed in the view of obtaining green nano-chemical devices.

Keywords: molecular machines, light activated lights, partition functions, thermodynamically functions, path integrals.

Acknowledgment. We hereby acknowledge the research project PED123/2017 of UEFISCDI-Romania.

GREEN-NANOCHEM **2018**
7 June, Timişoara
West University of Timişoara
*NEW FRONT CHEM 27 (**2018**) 37-49*

PREPARATION AND CHARACTERIZATION OF NANO CHITOSAN

***PAHOMI Alexandru*[1,2], *VLAD-OROS Beatrice*[1,2♣], *DASCĂLU Daniela*[1,2]**

[1]*Department of Biology-Chemistry, West University of Timisoara, Timisoara, Romania;*
[2]*Advanced Environmental Research Laboratories, West University of Timisoara, Romania,* ♣*e-mail: beatrice.vlad@e-uvt.ro*

Chitosan is a partially deacetylated polymer that can be obtained through alkaline deacetylation of chitin and consists of a β-(1,4)-linked-D-glucosamine residue with the amine groups randomly acetylated [1, 2].

The preparation and characterization of chitosan nanostructures is reviewed because, compared to traditional micro-sized supports, nano-sized adsorbents possess good performance due to small size, high specific surface area and quantum size effect [3].

As methods taken into account, we reviewed the emulsion method, ionic gelation method, reverse micellar method, and also the main techniques used for the physicochemical characterization of nano chitosan particles (FT-IR, XRD, SEM, AFM, TGA and DSC) [4, 5, 6].

Keywords: chitosan, preparation methods, nano adsorbents, physicochemical characterization

References

[1] A. Grenha, "Chitosan nanoparticles: A survey of preparation methods," *J. Drug Target.*, vol. 20, no. 4, pp. 291–300, 2012.
[2] L. M. Zhao *et al.*, "Preparation and application of chitosan nanoparticles and nanofibers," *Brazilian J. Chem. Eng.*, vol. 28, no. 3, pp. 353–362, 2011.
[3] T. Banerjee, S. Mitra, A. Kumar Singh, R. Kumar Sharma, and A. Maitra, "Preparation, characterization and biodistribution of ultrafine chitosan nanoparticles," *Int. J. Pharm.*, vol. 243, no. 1–2, pp. 93–105, 2002.
[4] H. Katas and H. O. Alpar, "Development and characterisation of chitosan nanoparticles for siRNA delivery," *J. Control. Release*, vol. 115, no. 2, pp. 216–225, 2006.
[5] M. S. Sivakami, T. Gomathi, J. Venkatesan, H. S. Jeong, S. K. Kim, and P. N. Sudha, "Preparation and characterization of nano chitosan for treatment wastewaters," *Int. J. Biol. Macromol.*, vol. 57, pp. 204–212, 2013.
[6] Y. Ohya, M. Shiratani, H. Kobayashi, and T. Ouchi, "Release behavior of 5-fluorouracil from chitosan-gel nanospheres immobilizing 5-fluorouracil coated with polysaccharides and their cell specific cytotoxicity," *J. Macromol. Sci. Part A*, vol. 31, no. 5, pp. 629–642, 1994.

Acknowledgements –This work was supported by the grant PN3-P3-285, Polymeric NanoBioMaterials for drug delivery: developing and implementation of safe-by-design concept enabling safe healthcare solutions.