UNIVERSITATEA DE VEST DIN TIMIŞOARA
CBG
FACULTATEA DE
CHIMIE, BIOLOGIE, GEOGRAFIE

LABORATORUL DE CERCETARE ÎN

CHIMIE-FIZICĂ STRUCTURALĂ ȘI COMPUTAȚIONALĂ PENRU NANOȘTIINȚE ȘI QSAR (CF-SC-NQ)

PREZENTARE UVT/ Octombrie 2013

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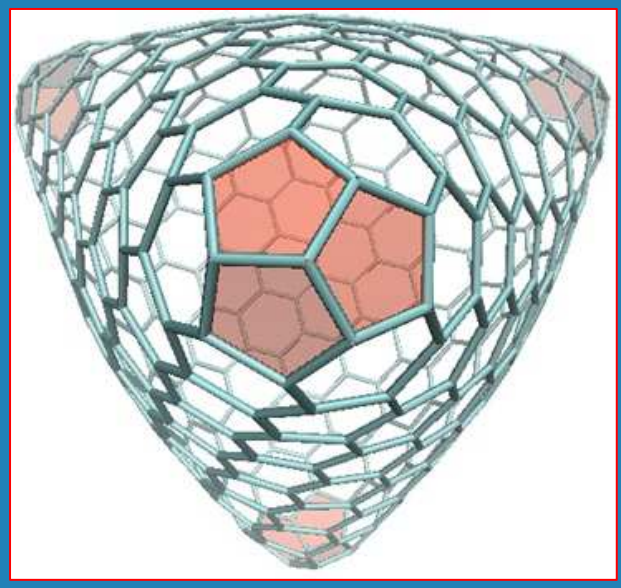
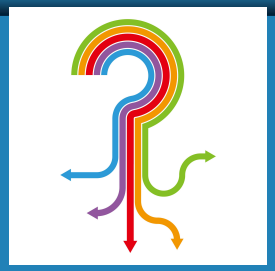
http://www.mvputz.iqstorm.ro/cercetare.php



Motivație:
Abordarea a 3 dintre
Problemele Majore ale Omenirii

ENERGIE SIGURĂ, ECOLOGICĂ ȘI EFICIENTĂ



TRANSPORTUL ECOLOGIC ȘI COMUNICAREA INTELIGENTĂ

VIAȚĂ MAI LUNGĂ Și MAI SĂNĂTOASĂ

FET H2020 Proactive WP2014-15 working list

European Commission

DRAFT

Time for Time

Health, Demographic Change and Wellbeing

Micro- and nanoelectronics

Knowing, doing, being

European Bio-Economy Challenges

Advanced materials

Adaptive Bottom-up Construction

Secure, clean and efficient energy

Global Systems Science

Industrial biotechnology

Constructive Symbiosis

Smart, green and integrated transport

Photonics

Ecological technology

Climate action, resource efficiency and raw materials

Nanotechnology

Nano-bio-chem interface

Europe in a changing world

Exploiting light-matter interaction

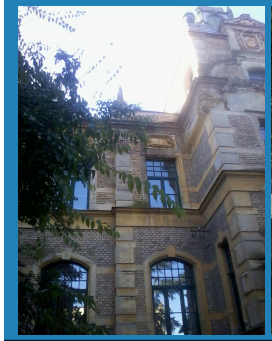
Advanced Manufacturing

Secure societies

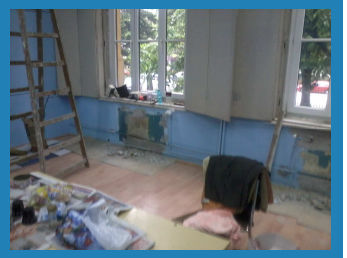
Quantum technologies

http://cordis.europa.eu/fp7/ict/fet-proactive/fetconsult2012-topics_en.html

1. MISIUNE, LOCAȚIE

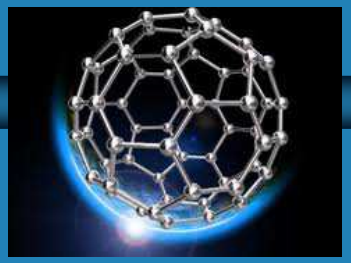


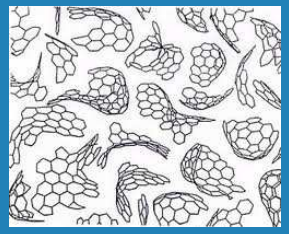
L-CF-SC-NO este o unitate de cercetare ştiinţifică avansată şi independentă, fără personalitate juridică, în DOMENIUL FUNDAMENTAL: ȘTIINȚE NATURALE ȘI MATEMATICE, cu obiective de cercetare fundamentală, diseminare, educație, dezvoltare și de promovare instituțională la nivelul CHIMIEI MULTIDISCIPLINARE (*incluzând nelimitativ disciplinele de chimie-fizică, chimie informatică, chimie matematică, chimie organică-fizică, chimie nano-anorganică, chimie-biologie, biochimie, biologie informatică, chimie farmaceutică, chimie medicală, ecotoxicologie, geochimie, QSAR*, etc.) aplicată fenomenelor și proprietăților NANO-STRUCTURALE ale materiei, în stare izolată și în interacție reciprocă și cu mediul (QS[A-activity/P-property/T-toxicity]R), explicate și controlate de legile FIZICII, cu suport MATEMATIC și COMPUTAȚIONAL.

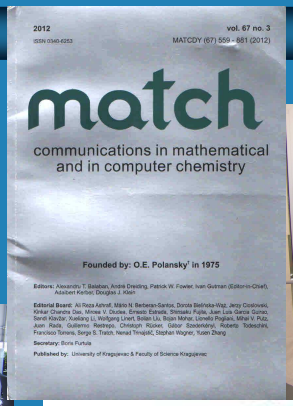


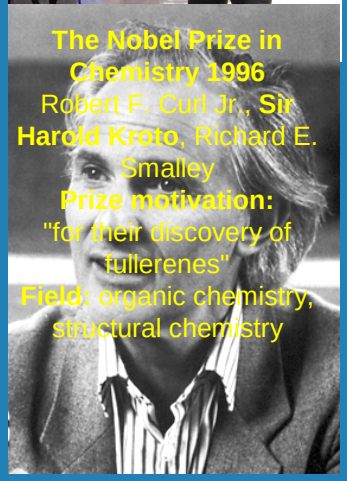
2. ÎNSEMN, ȘI…ISTORIE PRE-FONDATOARE

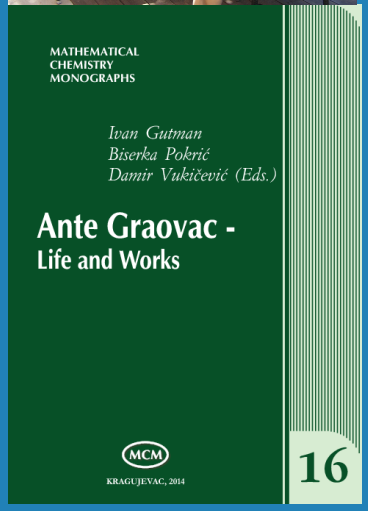
Spațiul fullerenelor icosaedrale largi de tipul C240. Structura a fost obținută computațional prin mecanismul gSW+2sBerge (transformare topologică generalizată de tip Stone-Wales la care se adaugă aplicarea teoremei Berge de transformare a spațiului de isomeri în el însuși, aici limitată la transformarea topologică implicând două legături chimice din structură, pe scurt *G=2s(H)*), completetând astfel (inovator) limitarea algoritmului Fowler-Manolopoulos de generare spiralată de inele penta-hexagonale în fullerenele și nanotuburile "clasice".

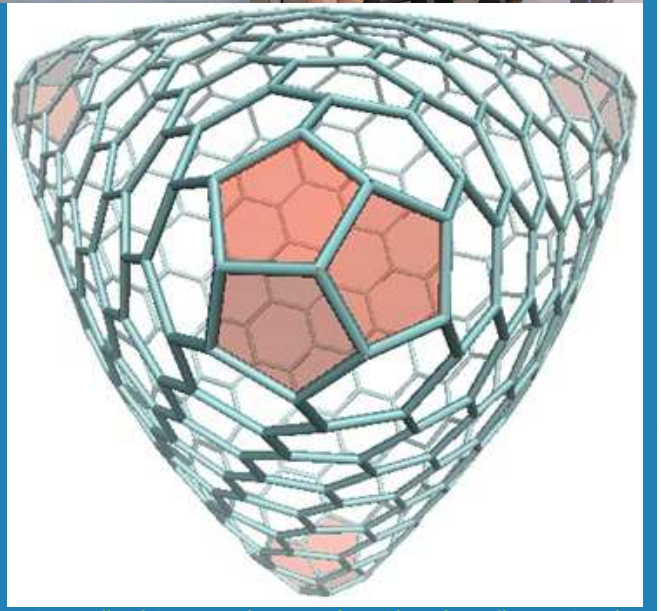










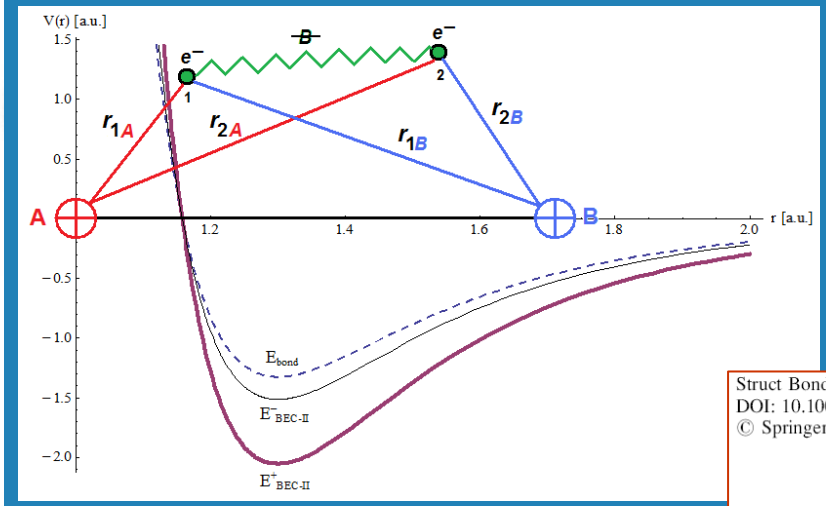


Generalized Stone-Wales Transformations for Fullerene Graphs Derived from Berge's Switching Theorem
Ottorino Ori, Mihai V. Putz, Ivan Gutman, și Peter Schwerdtfeger

3. PROGRAM-CADRU/STRATEGIE, DIRECȚII ȘI TEME DE CERCETARE

Abordarea "bosonică" a materiei și a legăturii chimice în special

$$\left\langle \hat{H}_{FB} \right\rangle = \left\langle \hat{H}_{F} \right\rangle_{\substack{FERMIONIC \\ SIDE}} + \left\langle \hat{H}_{B} \right\rangle_{\substack{BOSONIC \\ SIDE}}$$



$$N = \int \rho(\mathbf{r})d\mathbf{r} = \int \left|\psi(\mathbf{r})\right|^2 d\mathbf{r}$$

$$m_B = \frac{\hbar^2}{2}\frac{(2\pi n+1)^2}{E_{bond}X_{bond}^2}$$

Struct Bond (2012) 149: 1–50
DOI: 10.1007/978-3-642-32753-7_1
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Density Functional Theory of Bose–Einstein Condensation: Road to Chemical Bonding Quantum Condensate

Mihai V. Putz

Int. J. Mol. Sci. **2010**, *11*, 4227-4256; doi:10.3390/ijms11114227

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International Journal of
Molecular Sciences
ISSN 1422-0067
www.mdpi.com/journal/ijms

Article

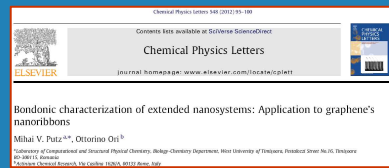
The Bondons: The Quantum Particles of the Chemical Bond

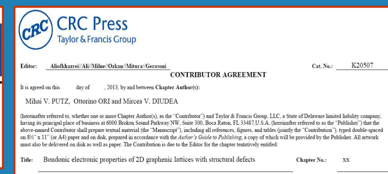
Mihai V. Putz [1,2]

[1] Laboratory of Computational and Structural Physical Chemistry, Chemistry Department, West University of Timişoara, Pestalozzi Street No.16, Timişoara, RO-300115, Romania; E-Mail: mvputz@cbg.uvt.ro or mv_putz@yahoo.com; Tel.: ++40-256-592-633; Fax: ++40-256-592-620; Web: www.mvputz.iqstorm.ro

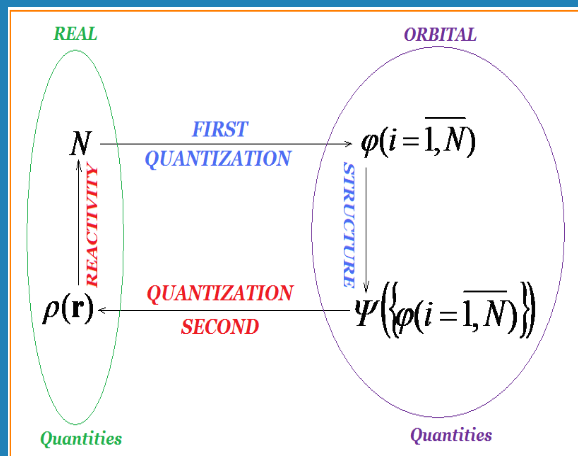
[2] Theoretical Physics Institute, Free University Berlin, Arnimallee 14, 14195 Berlin, Germany

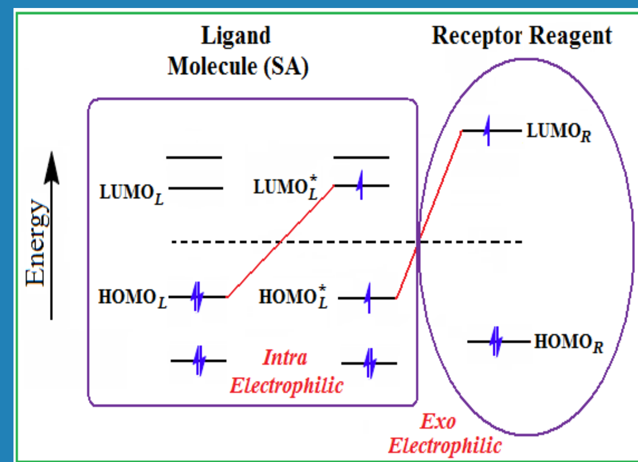
3. PROGRAM-CADRU/STRATEGIE, DIRECȚII ȘI TEME DE CERCETARE


Chemical Physics Letters 546 (2012) 95–100
Contents lists available at SciVerse ScienceDirect
Chemical Physics Letters
journal homepage: www.elsevier.com/locate/cplett
Bondonic characterization of extended nanosystems: Application to graphene's nanoribbons
Mihai V. Putz [a,*], Ottorino Ori [b]

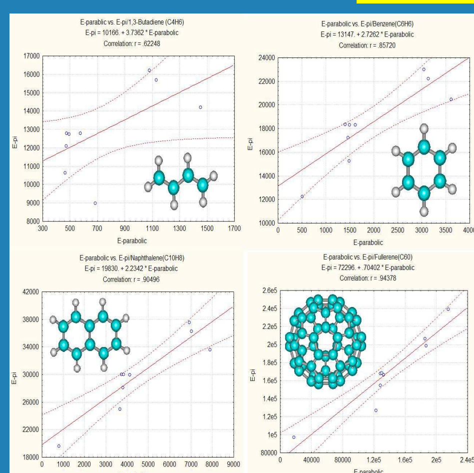

CRC Press
Taylor & Francis Group
CONTRIBUTOR AGREEMENT
Mihai V. PUTZ, Ottorino ORI and Mircea V. DIUDEA
Title: Bondonic electronic properties of 2D graphenic lattices with structural defects

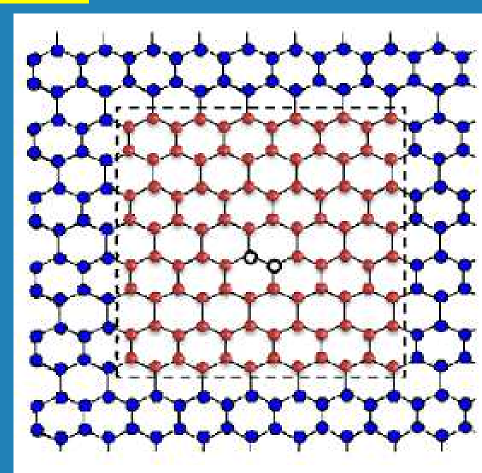
Abordarea cuantică a reactivității chimice

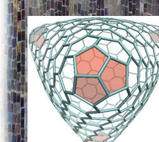




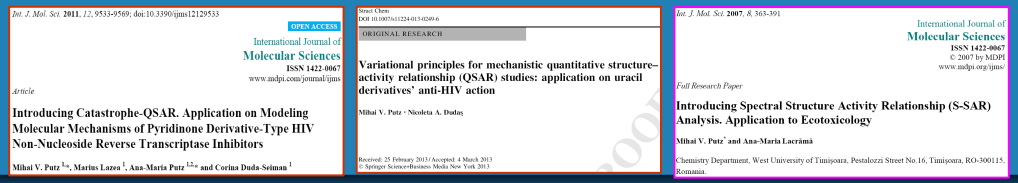
$$E_{par(abolic)} \cong -\chi N_\pi + \eta N_\pi^2$$







3. PROGRAM-CADRU/STRATEGIE, DIRECȚII ȘI TEME DE CERCETARE


Int. J. Mol. Sci. 2011, 12, 9533-9569; doi:10.3390/ijms12129533
OPEN ACCESS
International Journal of Molecular Sciences
ISSN 1422-0067
www.mdpi.com/journal/ijms
Article
Introducing Catastrophe-QSAR. Application on Modeling Molecular Mechanisms of Pyridinone Derivative-Type HIV Non-Nucleoside Reverse Transcriptase Inhibitors
Mihai V. Putz [1,*], Marius Lazea [1], Ana-Maria Putz [1,2,*] and Corina Duda-Seiman [1]

Struct Chem
DOI 10.1007/s11224-013-0249-6
ORIGINAL RESEARCH
Variational principles for mechanistic quantitative structure–activity relationship (QSAR) studies: application on uracil derivatives' anti-HIV action
Mihai V. Putz · Nicoleta A. Dudaș
Received: 25 February 2013 / Accepted: 4 March 2013
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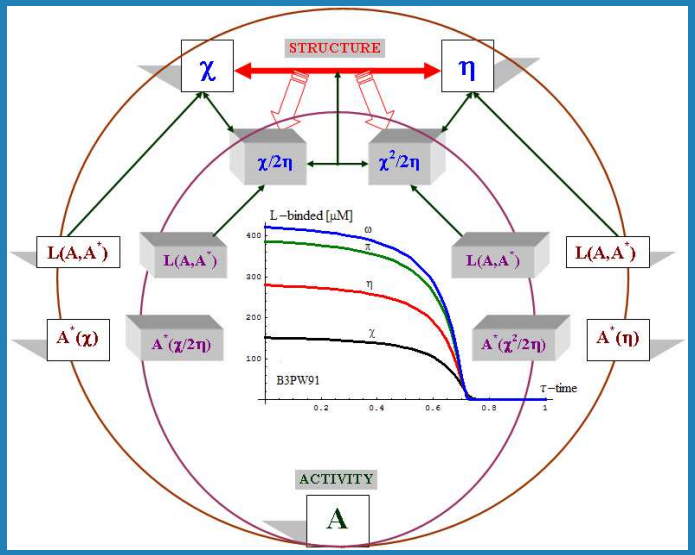
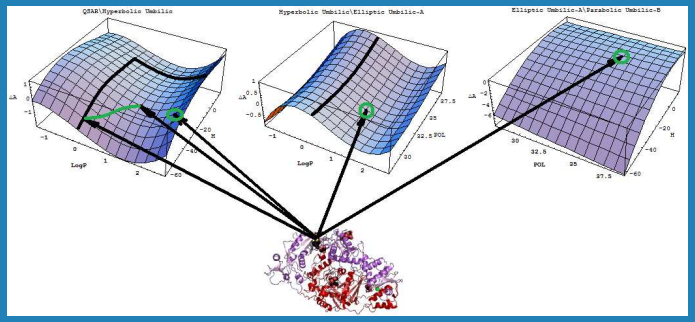
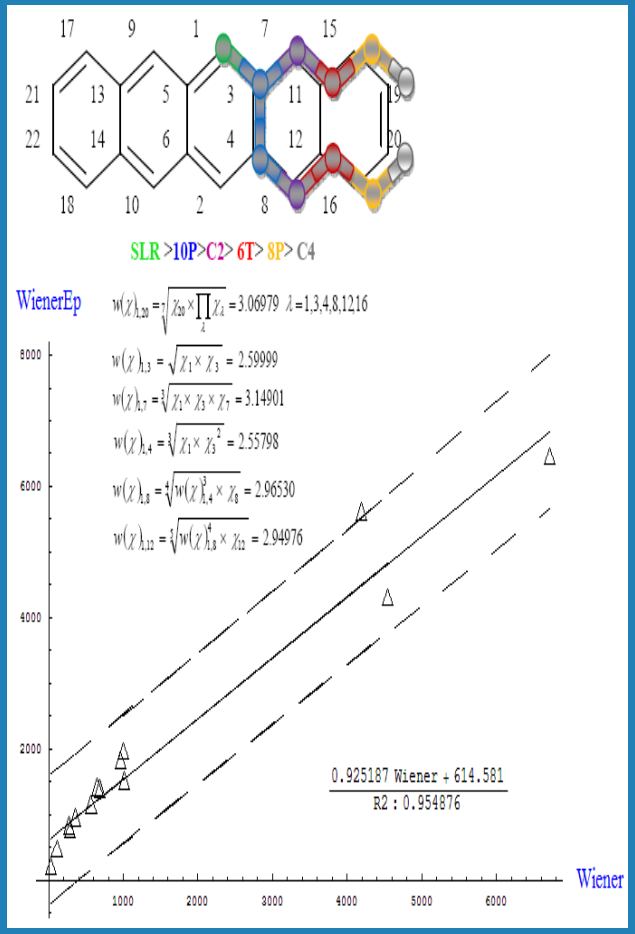
Int. J. Mol. Sci. 2007, 8, 363-391
International Journal of Molecular Sciences
ISSN 1422-0067
© 2007 by MDPI
www.mdpi.org/ijms/
Full Research Paper
Introducing Spectral Structure Activity Relationship (S-SAR) Analysis. Application to Ecotoxicology
Mihai V. Putz* and Ana-Maria Lacrămă
Chemistry Department, West University of Timişoara, Pestalozzi Street No.16, Timişoara, RO-300115, Romania.

Abordarea topologică și algebrică a interacției chimico-biologice și a toxicității







NANO-CHIMIA...
INFORMAȚIA FOTONICĂ...
TOXICOLOGIA CUANTICĂ...
APLICAȚII pentru SECOLUL XXI

To reduce the costs of lithium-ion batteries the automobile industry has changed from using lithium cobalt oxide to using less expensive lithium iron phosphate. When producing lithium iron phosphate by applying a microwave reactor the reaction time can be significantly reduced from hours down to minutes.

Inkjet printing technology, in which metallic nanoparticle suspensions are printed using ordinary commercial printers, is a promising technique for fabricating conductive lines for electronic applications

Zinc sulfide (ZnS) is one of the most important semiconductors. It has a great potential in several different technological applications such as in optoelectronic devices or as photonic crystals

Micelles are a classical example of nanostructures formed through the self-assembly of amphiphilic molecules in aqueous solvents.

What is special about nanomaterials?

When a particle becomes smaller, its surface becomes bigger relative to its volume, thus changing the overall properties of the resulting nanomaterial. It may be more reactive, have different optical, magnetic and electrical behavior, be mechanically stronger or more toxic compared to the same material on a larger scale. One major reason for these changes is that nanomaterials break a size barrier below which quantum effects can begin to dominate their behavior.

Nanomedicine

“Nano” in Everyday Products

Surface-active additives adsorb at the air/liquid or liquid/liquid interface, often building a monolayer with a thickness of only a few nanometers.

The stability and properties of these products depend on surfactants which either occur naturally or are used as additives. Supplements like omega-3 fatty acids are often encapsulated in nanostructures to prevent food tasting fishy.

the perfect “crema“ and foam

Nano-electrotechnology

nanodrugs

Nanocomposites in packaging materials are used to extend the life of food and drinks by inhibiting bacterial growth or strengthening the barrier for carbon dioxide and oxygen.

Nanotechnology further assists in producing memory chips with remarkably increased disk space. Nanoparticles are investigated for new developments in photovoltaic systems, such as thin-layer solar cells, dye solar cells or polymer solar cells.

Alkane thiol-anchored self-assembled monolayers on gold are widely used to immobilize and detect molecules, including DNA, which become covalently bonded to the SAM (self-assembly monolayers) on the gold surface.

hydrogen storage

Microemulsions are made of at least two immiscible fluids plus a surfactant. High surfactant content influences the skin barrier and allows the active ingredients which are dissolved in the microemulsions to move through the skin into the organism.

Polymer-carbon black composites are viscoelastic materials that consist of carbon black clusters inducing dielectric properties which are dispersed in a polymeric matrix.

A new technique referred to as silicon ink technology remarkably reduces the production costs of solar cells. This technique is based on a special ink that contains dispersed silicon nanoparticles.

drug delivery

Nanoscale coatings of organic silanes or thiols with functional end-groups are a smart procedure to tune material surface properties without changing the material thickness.

polymer-carbon black

carbon nanotubes

Nanocatalysis

3. PROGRAM-CADRU/STRATEGIE, DIRECȚII ȘI TEME DE CERCETARE

$$IQ_{Obs/Free} = \frac{\left(\frac{Particle}{Wave}\right)_{\substack{Observed\\Evolution}}}{\left(\frac{Particle}{Wave}\right)_{\substack{Free\\Evolution}}} = \sqrt{\frac{3-2n^2}{3+2n^2}}\exp\left(\frac{2n^2}{9-4n^4}\right)$$

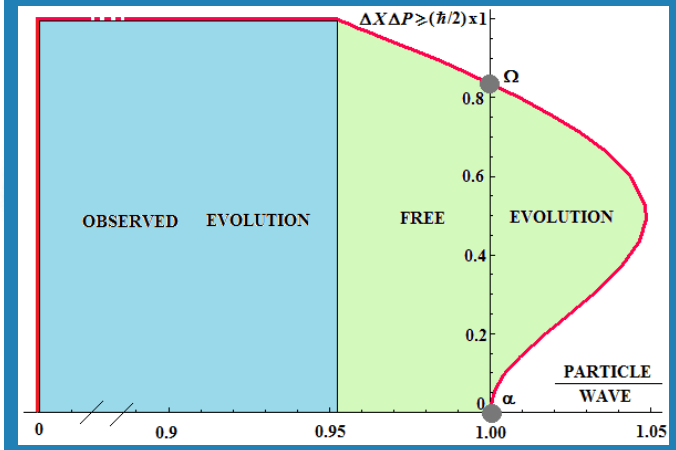
NANO-CHIMIE-FIZICĂ CUANTICĂ

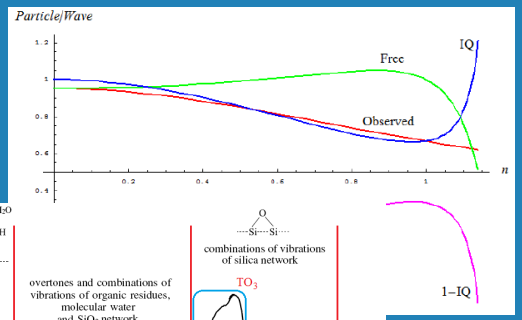
$$n \to n_{Obs} = \sqrt{\frac{\langle x_0^2\rangle_{Exp}}{\left|\langle x^2\rangle_{Exp} - \langle x_0^2\rangle_{Exp}\right|}}$$

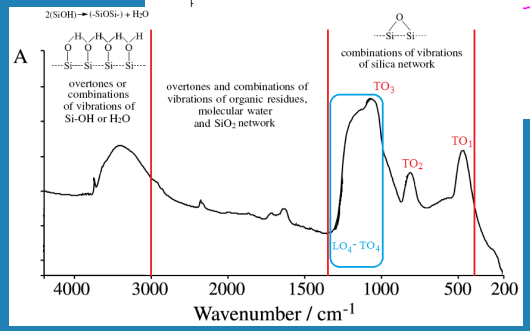
$$n \to n_{Free} = \sqrt{\frac{\langle x_0^2\rangle_{Exp}}{\left|\langle x^2\rangle_{Exp} + \langle x_0^2\rangle_{Exp}\right|}}$$

$$n_{Obs} = \frac{1}{\tilde{\upsilon}_0\sqrt{\frac{1}{\Delta\tilde{\upsilon}^2_{FWHM}} + \frac{1}{4}\left(\frac{1}{\tilde{\upsilon}_L^2} + \frac{1}{\tilde{\upsilon}_R^2} + \frac{2}{\tilde{\upsilon}_L\tilde{\upsilon}_R}\right) - \frac{1}{\tilde{\upsilon}_0^2}}}$$

$$n_{Free} = \frac{1}{\tilde{\upsilon}_0\sqrt{\frac{1}{\Delta\tilde{\upsilon}^2_{FWHM}} + \frac{1}{4}\left(\frac{1}{\tilde{\upsilon}_L^2} + \frac{1}{\tilde{\upsilon}_R^2} + \frac{2}{\tilde{\upsilon}_L\tilde{\upsilon}_R}\right) + \frac{1}{\tilde{\upsilon}_0^2}}}$$







$$\Delta x\Delta p \geq \frac{\hbar}{2}\sqrt{1-n^2}$$

$$n \in [0,1]$$

$$n = \sqrt{\frac{\langle x_0^2\rangle_{Exp}}{\left|\langle x^2\rangle_{Exp} - \langle x_0^2\rangle_{Exp}\right|}}$$

Int. J. Mol. Sci. **2010**, *11*, 4124-4139; doi:10.3390/ijms11104124

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International Journal of **Molecular Sciences**

ISSN 1422-0067

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Article

On Heisenberg Uncertainty Relationship, Its Extension, and the Quantum Issue of Wave-Particle Duality

Mihai V. Putz [1,2]

Int. J. Mol. Sci. **2012**, *13*, 15925-15941; doi:10.3390/ijms131215925

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International Journal of **Molecular Sciences**

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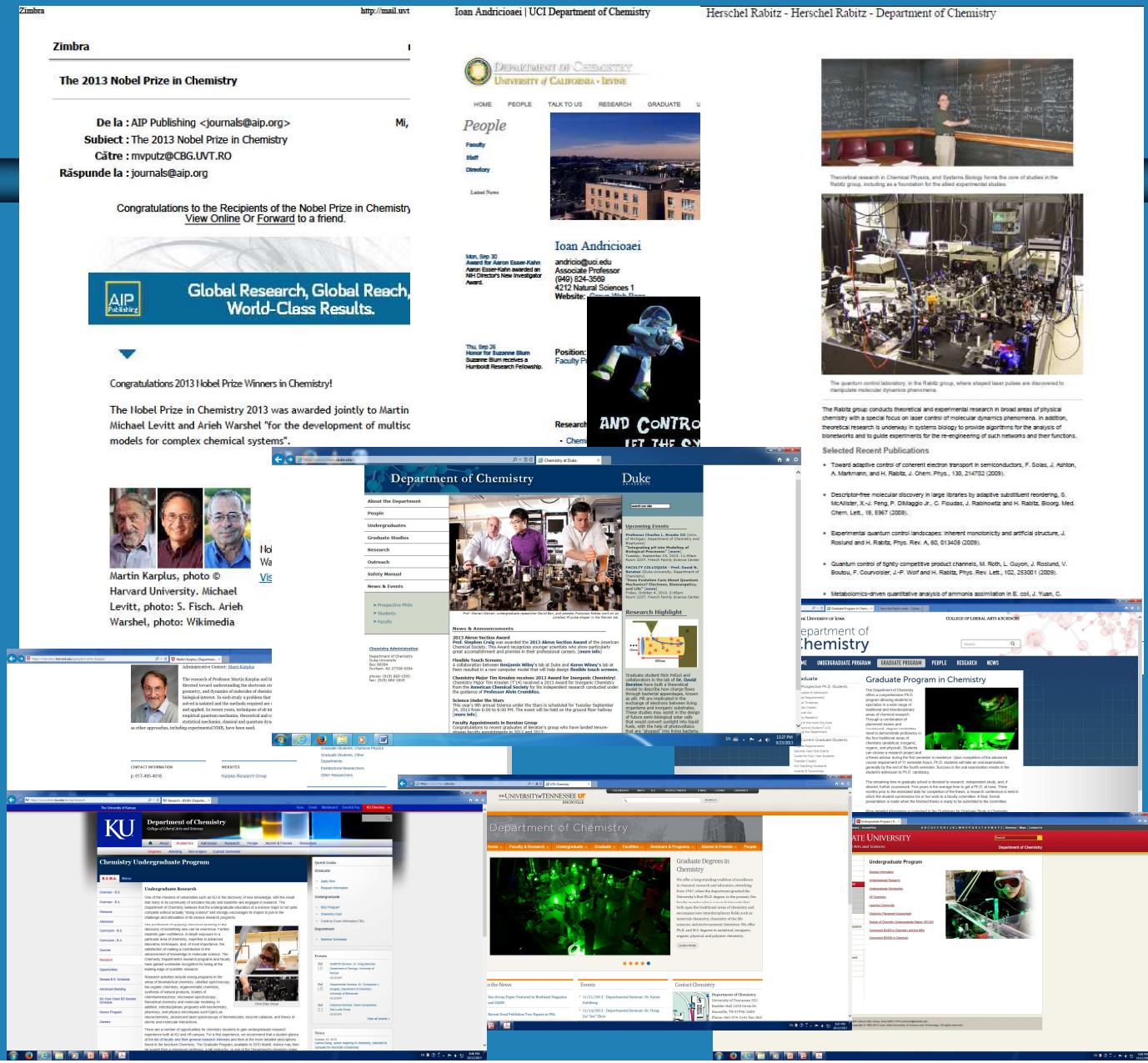
Article

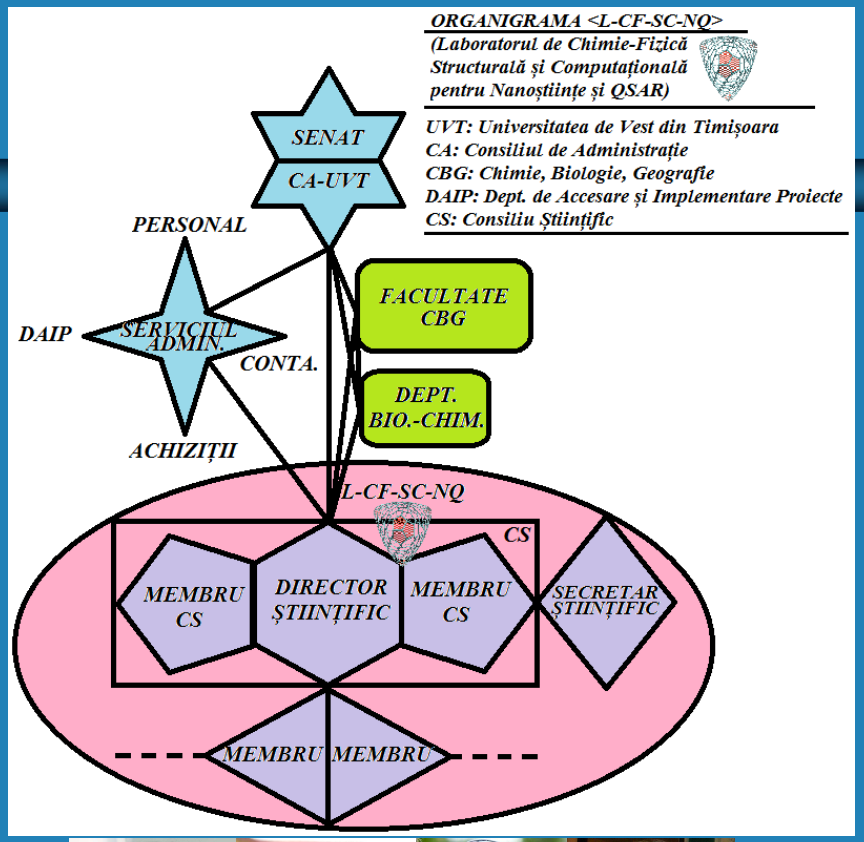
Spectral Inverse Quantum (Spectral-IQ) Method for Modeling Mesoporous Systems: Application on Silica Films by FTIR

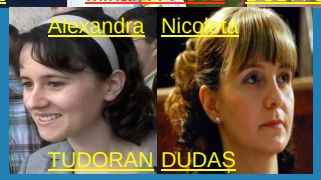
Ana-Maria Putz [1,2] **and Mihai V. Putz** [2,*]

RECUNOAȘTEREA FIZICII & MODELĂRII CUANTICE ÎN LUMEA...CHIMIEI



4. ORGANIZARE ȘI ORGANIGRAMĂ
Componența curentă (și recentă) a L-CF-SC-NQ



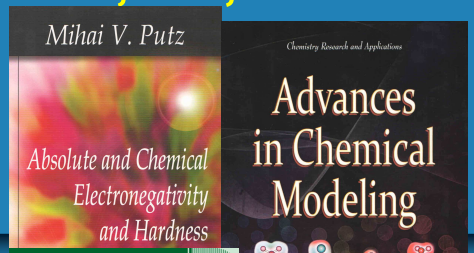


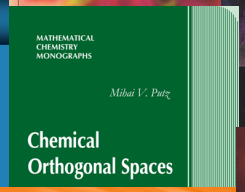
Foști membri:

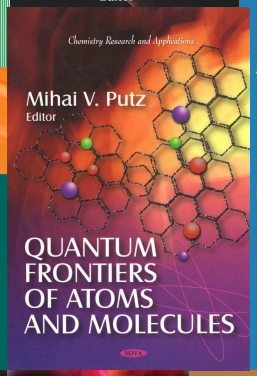
CV-ul Directorului Ştiinţific al L-CF-SC-NQ

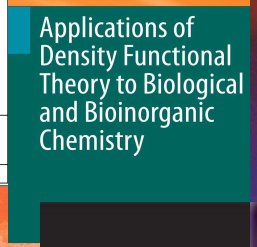
FIŞA DE VERIFICARE PENTRU ÎNDEPLINIREA STANDARDELOR MINIMALE NECESARE ŞI OBLIGTORII
PENTRU ***CONFERIREA TITLULUI DIDACTIC DE "PROFESOR UNIVERSITAR"***
ÎN DOMENIUL ***~CHIMIE~***[1]
SYNÓPSIS

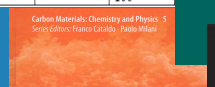
Crt.	Domeniul Activităţilor	Punctaj pe activitate	Tipul Activităţilor	REALIZĂRI pe Categorii şi Restricţii		PUNCTAJ REALIZĂRI Σ'Activităţi		PUNCTAJ NECESAR Σ'Activităţi
A1	*Activitate Didactică /profesională*	3	Cărţi sau capitole de carte	**Total Cărţi & Capitole** (minim 3):	67	201		9
				Prim Autor (minim 1):	56			
A2	*Activitate Cercetare*	1	Articole in reviste cotate ISI Thomson Reuters	**Total Articole ISI** (minim 35):	58	58	78	41
				În reviste Intl. (minim 23)	47			
				Factor de Impact cumulat (minim 40 ISI):	115.232			
				Autor principal (minim 10 ca prim sau correspondent):	56			
		4	Granturi/proiecte NAŢIONALE câştigate prin competiţie	**Director** (minim 1):	2	8		
		2		**Ca Membru** (minim 1):	6	12		
A3	*Recunoaşterea impactului activităţii*	0.5	Citări in reviste ISI şi BDI	**Total ISI & BDI** (Minim 100):	267	133.5		50
				GRAND TOTAL		412.5		100

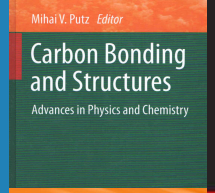


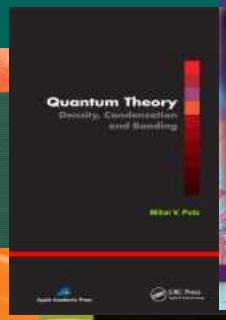


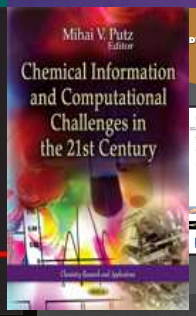


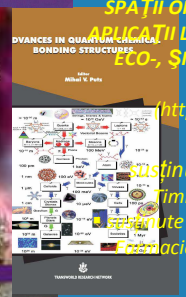


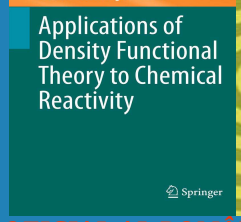


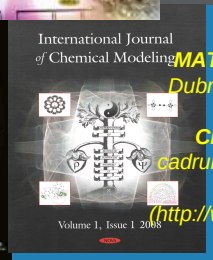












Publicaţii
în Jurnale şi Cărţi internaţionale de prim rang:
- *Physical Review E*
- *Journal of Physical Chemistry A*
- *Int. Journal of Quantum Chemistry*
- *Journal of Computational Chemistry*
- *Theoretical Chemistry Accounts*
- *Int. Journal of Molecular Sciences*
- *J. Theor. Comp. Chemistry*
- *MATCH Comm. Math. Comput. Chem.*
- *J. of Molecular Structure: THEOCHEM*
- *Journal of Mathematical Chemistry*
- *Molecules*
- *Chemistry Central Journal*
- *Chemical Physics Letters*
- *Structure and Bonding*

Proiecte internaţionale:
STOCHASTIC ANALYSIS OF THE OPEN SYSTEMS WITH THE FOKKER-PLANCK EQUATION BY PATH INTEGRALS; *grant DAAD 322 A/04/17690, Institute of Theoretical Physics, Free University of Berlin (2004);*

▪***BOSE-EINSTEIN CONDENSATION IN RANDOM POTENTIALS;*** *Center for International Cooperation (CIC), Institute of Theoretical Physics, Free University of Berlin (2010);*

▪***DENSITY FUNCTIONAL THEORY OF BOSE-EINSTEIN CONDENSATION FOR THE QUASIHOMOGENEOUS SYSTEMS;*** *grant DAAD 322A/11/05356, Institute of Theoretical Physics, Free University of Berlin (2011).*

Proiecte naţionale:
UNIFICAREA CUANTICĂ A LEGĂTURII CHIMICE PRIN FUNCŢIONALA DENSITATE A ELECTRONEGATIVITĂŢII ŞI FUNCŢIA DE LOCALIZARE ELECTRONICĂ CU APLICAŢII LA REACTIVITATEA NANO-SISTEMELOR NATURALE COMPLEXE; *grant CNCSIS: AT54/2006-2007*

▪***CUANTIFICAREA LEGĂTURII CHIMICE ÎN SPAŢII ORTOGONALE DE REACTIVITATE. APLICAŢII LA MOLECULE DE INTERES BIO-, ECO-, ŞI FARMACO-LOGIC;*** *grant CNCS-UEFISCDI: TE16/2010-2013 (http://mvputz.iqstorm.ro/g1.php).*

Doctorate Tutorate:
Susţinute la Universitatea de Vest din Timişoara, ***2007, 2009, 2010, 2011****;*
Susţinute la Universitatea de Medicină şi Farmacie "Victor Babeş" din Timişoara, ***2010, 2012***

Manifestări ştiinţifice co-organizate
MATH/CHEM/COMP, *Inter-University Centre, Dubrovnik, Croatia, ediţiile XXIII (2008) –XXVI (2011) (http://mcc.irb.hr)*
Chemical Modelling *(Symposium no. 2) în cadrul* ***ICCMSE****, 02-07 October 2011, Halkidiki, Greece (http://www.iccmse.org/Sessions_Minisymposia.htm)*

[1] *Conform cu MONITORUL OFICIAL AL ROMÂNIEI, PARTEA I, Nr. 890 bis/27.XII.2012, PAG.9 (Anexa 4, la zi valabilă)*

Colaborări ale Directorului CF-SC-NQ

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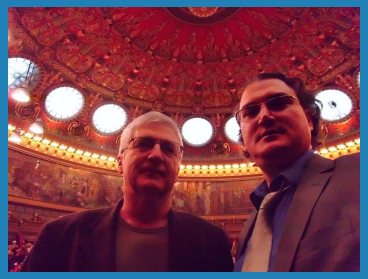

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Prof. Emilia Sicilia
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Premii și Granturi ale Directorului CF-SC-NQ

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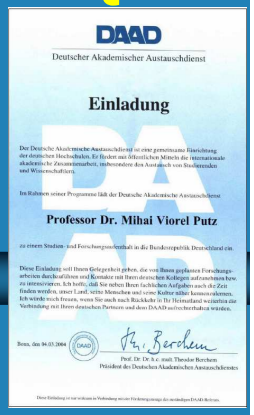
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Einladung

Professor Dr. Mihai Viorel Putz

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PREMIUL

"Pentru TÂNĂRUL CERCETĂTOR EMINENT AL TIMIȘOAREI"

Se acordă domnului conf. univ. dr. MIHAI VIOREL PUTZ, Departamentul de Chimie, Universitatea de Vest din Timișoara

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Premiul I

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Universitatea de Vest, Timișoara
Secțiunea Cercetătorul anului

03 Noiembrie 2010

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