

LISTA DE LUCRĂRI

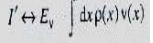
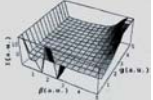
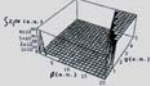
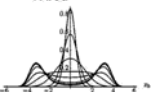
SYNOPSIS:

(i) TEZA DE DOCTORAT SI TEZA DE ABILITARE	2
(ii) ARTICOLE ISI THOMPSON REUTERS	3
(iii) ARTICOLE IN INTERNATIONAL PROCEEDINGS	21
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(i) TEZA DE DOCTORAT SI TEZA DE ABILITARE

Informații Teza de Doctorat	Data Susținerii
PUTZ M.V. <i>CONTRIBUȚII LA TEORIA FUNCȚIONALEI DENSITATE CU APLICAȚII ÎN TEORIA REACTIVITĂȚII CHIMICE ȘI A ELECTRONEGATIVITĂȚII</i> Universitatea de Vest din Timișoara publicată ulterior în limba Engleză <i>Contributions within Density Functional Theory with Applications to Chemical Reactivity Theory and Electronegativity</i> în versiune extinsă la Dissertation. Com, Parkland, Florida, USA (2003) pag. 180; ISBN: 1-58112-184-9; ♣URL: www.dissertation.com/book.php?method=ISBN&book=1581121849	2002 15 Martie
Informații Teza de Abilitare	Data Susținerii
PUTZ M.V. <i>CHEMICAL ORTHOGONAL SPACES OF ATOMS AND MOLECULES</i> Universitatea Babes-Bolyai din Cluj-Napoca și publicată în volumul cu titlul <i>Chemical Orthogonal Spaces</i> în seria Mathematical Chemistry Monographs, Vol. 14, University of Kragujevac, Serbia (2012), X + pp. 240 Hardcover, 12 color illus.; ISBN: 978-86-6009-019-7; ♣URL: http://www.pmf.kg.ac.rs/match/mcm14.html	2013 20 Martie

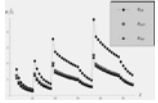
(ii) ARTICOLE ISI THOMPSON REUTERS

Nr.	Articol	FACTOR DE IMPACT cel mai bun: valoarea pe 2015/2016 sau media pe ultimii 4/5 ani sau în anul publicării (precum disponibil) ABSTRACT GRAFIC
1.	PUTZ M.V., CHIRIAC A., MRACEC M. Models of Photomobility Selectivity in Rare Gas Matrices <i>Revue Roumaine de Chimie</i> 46(2) (2001) 153-160	0.250/ ¹ 2015/2016 
2.	PUTZ M.V., CHIRIAC A., MRACEC M. Foundations for a Theory of the Chemical Field. I. General Aspects <i>Revue Roumaine de Chimie</i> 46(4) (2001) 387-393; dedicated to Professor Dr. Alexandru T. Balaban, member of the Romanian Academy, on the occasion of his 70 th anniversary	0.250/ ² 2015/2016 
3.	PUTZ M.V., CHIRIAC A., MRACEC M. Foundations for a Theory of the Chemical Field. II. The Chemical Action <i>Revue Roumaine de Chimie</i> 46(10) (2001) 1175-1181	0.250/ ³ 2015/2016 
4.	PUTZ M.V., CHIRIAC A., MRACEC M. Foundations for a Theory of the Chemical Field. III. The Integrated Electronegativity <i>Revue Roumaine de Chimie</i> 47(1-2) (2002) 201-206; dedicated to the memory of Professor I.G. Murgulescu	0.250/ ⁴ 2015/2016 
5.	KLEINERT H., PELSTER A., PUTZ M.V. Variational Perturbation Theory for Markov Processes <i>Physical Review E</i> 65(6) (2002) 066128/1-7; DOI: 10.1103/PhysRevE.65.066128 ♣ URL: http://link.aps.org/abstract/PRE/v65/e066128 ; ♣ URL: http://arxiv.org/abs/cond-mat/0202378	2.252/ ⁵ 2015/2016 

¹ <http://www.bioxbio.com/if/html/REV-ROUM-CHIM.html>² <http://www.bioxbio.com/if/html/REV-ROUM-CHIM.html>³ <http://www.bioxbio.com/if/html/REV-ROUM-CHIM.html>⁴ <http://www.bioxbio.com/if/html/REV-ROUM-CHIM.html>⁵ <http://www.bioxbio.com/if/html/PHYS-REV-E.html>

6. **PUTZ M.V., RUSSO N., SICILIA E.**
Atomic Radii Scale and Related Size Properties from Density Functional
Electronegativity Formulation
Journal of Physical Chemistry A
107(28) (2003) 5461-5465; DOI: 10.1021/jp027492h
♣ URL: <http://pubs.acs.org/doi/abs/10.1021/jp027492h?prevSearch=&searchHistoryKey>

2.883/⁶
2015/2016



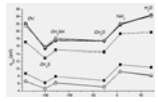
7. **PUTZ M.V.**
Electronic Density from Structure Factor Determination in Small Deformed
Crystals
International Journal of Quantum Chemistry
94(4) (2003) 222-231
DOI: 10.1002/qua.10475
♣ URL: <http://onlinelibrary.wiley.com/doi/10.1002/qua.10475/abstract>

2.184/⁷
2015/2016



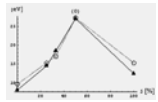
8. **PUTZ M.V., RUSSO N., SICILIA E.**
On the Application of the HSAB Principle through the Use of Improved
Computational Schemes for Chemical Hardness Evaluation
Journal of Computational Chemistry, 25(7) (2004) 994-1003
DOI: 10.1002/jcc.20027
♣ URL: <http://onlinelibrary.wiley.com/doi/10.1002/jcc.20027/abstract>

3.648/⁸
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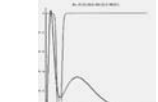
9. **PUTZ M.V., RUSSO N., SICILIA E.**
About the Mulliken Electronegativity in DFT
Theoretical Chemistry Accounts
114(1-3) (2005) 38-45; DOI: 10.1007/s00214-005-0641-4
♣ URL: <http://www.springerlink.com/content/r5q2791060262416/>
♣ URL: <http://arxiv.org/abs/physics/0405005>

1.806/⁹
2015/2016
2.115
5-Years



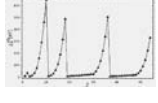
10. **PUTZ M.V.**
Markovian Approach of the Electron Localization Functions
International Journal of Quantum Chemistry
105(1) (2005) 1-11; DOI: 10.1002/qua.20645
♣ URL: <http://onlinelibrary.wiley.com/doi/10.1002/qua.20645/abstract>

2.184/¹⁰
2015/2016



11. **PUTZ M.V.**
Systematic Formulation for Electronegativity and Hardness and Their Atomic
Scales within Density Functional Softness Theory
International Journal of Quantum Chemistry
106(2) (2006) 361-389; DOI: 10.1002/qua.20787

2.184/¹¹
2015/2016



⁶ <http://pubs.acs.org/page/jpcafh/about.html>

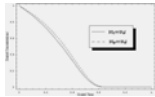
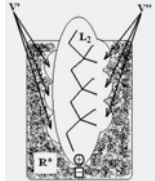
⁷ <http://www.bioxbio.com/if/html/INT-J-QUANTUM-CHEM.html>

⁸ <http://www.bioxbio.com/if/html/J-COMPUT-CHEM.html>

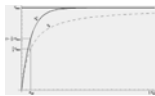
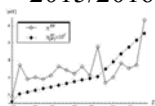
⁹ <http://www.bioxbio.com/if/html/THEOR-CHEM-ACC.html>

¹⁰ <http://www.bioxbio.com/if/html/INT-J-QUANTUM-CHEM.html>

¹¹ <http://www.bioxbio.com/if/html/INT-J-QUANTUM-CHEM.html>

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12. **PUTZ M.V., LACRĂMĂ A.-M., OSTAFE V.**
Full Analytic Progress Curves of the Enzymic Reactions in Vitro
International Journal of Molecular Sciences
7(11) (2006) 469-484; DOI: 10.3390/i7110469
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International Journal of Molecular Sciences
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DOI: 10.3390/i7110537
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Digest Journal of Nanomaterials and Biostructures
2(2) (2007) 207-219
♣ URL: http://www.chalcogen.ro/Putz-AntiHIV_DJNB_2007.pdf

 15. **PUTZ M.V., LACRĂMĂ A.-M.**
Enzymatic control of the bio-inspired nanomaterials at the spectroscopic level
Journal of Optoelectronics and Advanced Materials
9 (8) (2007) 2529 – 2534
♣ URL: <http://joam.inoe.ro/index.php?option=magazine&op=view&idu=858&catid=16>

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Introducing logistic enzyme kinetics
Journal of Optoelectronics and Advanced Materials
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♣ URL: <http://joam.inoe.ro/index.php?option=magazine&op=view&idu=931&catid=17>

 17. **PUTZ M.V.**
Semiclassical Electronegativity and Chemical Hardness
Journal of Theoretical and Computational Chemistry
6(1) (2007) 33-47
DOI: 10.1142/S0219633607002861


¹² <http://www.mdpi.com/journal/ijms>

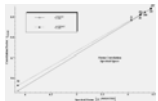
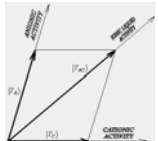
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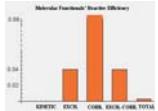
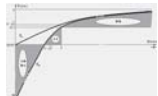
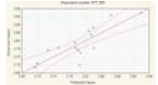
¹⁴ <http://www.bioxbio.com/if/html/DIG-J-NANOMATER-BIOS.html>

¹⁵ <http://www.bioxbio.com/if/html/J-OPTOELECTRON-ADV-M.html>

¹⁶ <http://www.bioxbio.com/if/html/J-OPTOELECTRON-ADV-M.html>

¹⁷ <http://www.bioxbio.com/if/html/J-THEOR-COMPUT-CHEM.html>

- ♣ URL: <http://www.worldscinet.com/jtcc/06/0601/S0219633607002861.html>
18. **PUTZ M.V., LACRĂMĂ A.-M.**
Introducing Spectral Structure Activity Relationship (S-SAR) Analysis.
Application to Ecotoxicology
International Journal of Molecular Sciences
8(5) (2007) 363-391; DOI: 10.3390/i8050363
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 19. **LACRĂMĂ A.-M., PUTZ M.V. (*), OSTAFE V.**
A Spectral-SAR Model for the Anionic-Cationic Interaction in Ionic Liquids:
Application to *Vibrio fischeri* Ecotoxicity
International Journal of Molecular Sciences
8(8) (2007) 842-863; DOI: 10.3390/i8080842
included in the Special Issue: Ionic Liquids (Jairton Dupont, guest editor)
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 20. **PUTZ M.V., PUTZ (LACRĂMĂ) A.-M.**
Spectral-SAR: Old Wine in New Bottle
Studia Universitatis Babeş-Bolyai - Seria Chimia
53 (2) (2008) 73-81
♣ URL: http://chem.ubbcluj.ro/~studiachimia/docs/Chimia_2_2008.pdf

 21. **PUTZ M.V.**
Density Functionals of Chemical Bonding
International Journal of Molecular Sciences
9(6) (2008) 1050-1095; DOI: 10.3390/ijms9061050
included in the Special Issue: Chemical Bond and Bonding (M.V. Putz, editor)
♣ URL: <http://www.mdpi.com/1422-0067/9/6/1050>

 22. **PUTZ M.V.**
Maximum Hardness Index of Quantum Acid-Base Bonding
MATCH Communications in Mathematical and in Computer Chemistry
60(3) (2008) 845-868
♣ URL: <http://www.pmf.kg.ac.rs/match/content60n3.htm>

 23. **VULPEŞ D., PUTZ M.V., CHIRIAC A.**
QSAR Study on The Anaesthetic Activity of Some Barbiturates and
Thiobarbiturates
Revue Roumaine de Chimie
54(9) (2009) 723-732


¹⁸ <http://www.mdpi.com/journal/ijms>

¹⁹ <http://www.mdpi.com/journal/ijms>

²⁰ <http://www.scijournal.org/impact-factor-of-STUD-U-BABES-BOL-CHE.shtml>

²¹ <http://www.mdpi.com/journal/ijms>

²² <http://www.bioxbio.com/if/html/MATCH-COMMUN-MATH-CO.html>

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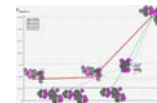
- ♣ URL: <http://web.icf.ro/rrch/>
24. **PUTZ M.V.**
Electronegativity: Quantum Observable
International Journal of Quantum Chemistry
109 (4) (2009) 733-738; DOI: 10.1002/qua.21957
♣ URL: <http://onlinelibrary.wiley.com/doi/10.1002/qua.21957/abstract>
25. **PUTZ M.V., PUTZ A.M., LAZEA M., IENCIU L., CHIRIAC A.**
Quantum-SAR Extension of the Spectral-SAR Algorithm. Application to Polyphenolic Anticancer Bioactivity
International Journal of Molecular Sciences
10(3) (2009) 1193-1214; DOI: 10.3390/ijms10031193
(Special Issue: Recent Studies on QSAR/QSPR Theory; E.A. Castro, editor)
♣ URL: <http://www.mdpi.com/1422-0067/10/3/1193>
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Chemical Action and Chemical Bonding
Journal of Molecular Structure: THEOCHEM
900 (1-3) (2009) 64-70; DOI: 10.1016/j.theochem.2008.12.026
♣ URL: <http://dx.doi.org/10.1016/j.theochem.2008.12.026>
27. **SELEGEAN M., PUTZ M.V. (*), RUGEA T.**
Effect of the Polysaccharide Extract from the Edible Mushroom *Pleurotus Ostreatus* against Infectious Bursal Disease Virus
International Journal of Molecular Sciences
10(8) (2009) 3616-3634; DOI: 10.3390/ijms10083616
♣ URL: <http://www.mdpi.com/1422-0067/10/8/3616>
28. **CHICU S.A., PUTZ M.V. (*)**
Köln-Timișoara Molecular Activity Combined Models toward Interspecies Toxicity Assessment
International Journal of Molecular Sciences
10(10) (2009) 4474-4497; DOI: 10.3390/ijms10104474
♣ URL: <http://www.mdpi.com/1422-0067/10/10/4474>
29. **PUTZ M.V.**
Path Integrals for Electronic Densities, Reactivity Indices, and Localization Functions in Quantum Systems
International Journal of Molecular Sciences
10(11) (2009) 4816-4940; DOI: 10.3390/ijms10114816

2.184/²⁴
2015/2016

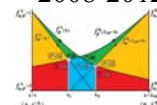
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$$P_{A \in \mathbb{R}} = \frac{\langle \psi_A | a | \psi_A \rangle}{\langle \psi_A | \psi_A \rangle}, \quad \langle \psi_A | \psi_A \rangle = 1$$

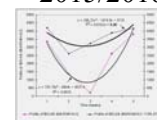
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2015/2016



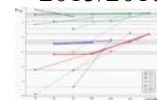
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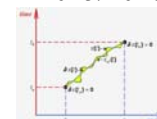
3.257/²⁷
2015/2016



3.257/²⁸
2015/2016



3.257/²⁹
2015/2016



²⁴ <http://www.bioxbio.com/if/html/INT-J-QUANTUM-CHEM.html>

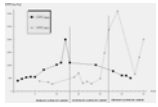
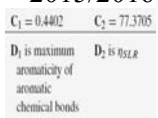
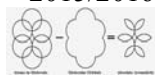
²⁵ <http://www.mdpi.com/journal/ijms>

²⁶ <http://www.bioxbio.com/if/html/J-MOL-STRUC-THEOCHEM.html>

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30. **PUTZ M.V., PUTZ A.M., LAZEA M., CHIRIAC A.** **0.619**^{/30}
Spectral vs. Statistic Approach of Structure-Activity Relationship. Application on **2015/2016**
Ecotoxicity of Aliphatic Amines
Journal of Theoretical and Computational Chemistry
8(6) (2009) 1235-1251; DOI: 10.1142/S0219633609005453
♣ URL: <http://www.worldscinet.com/jtcc/08/0806/S0219633609005453.html> 
31. **GHIJU S., PUTZ M.V. (*), CHIRIAC A.** **0.756**^{/31}
On Specific Vs. Non-Specific Enzymic Inter-Activity in Acute Myocardial **2015/2016**
Infarction
Digest Journal of Nanomaterials and Biostructures
5(2) (2010) 567-574
♣ URL: http://www.chalcogen.ro/567_Giju.pdf 
32. **PUTZ M.V.** **0.231**^{/32}
Chemical Hardness: Quantum Observable? **2010/2011**
Studia Universitatis Babeş-Bolyai - Seria Chemia
55 (2) –Tom I (2010) 47 – 50
♣ URL: <http://chem.ubbcluj.ro/~studiachemia/docs/Chemia22010t1.pdf> 
33. **TARKO L., PUTZ M.V. (*)** **1.056**^{/33}
On Electronegativity and Chemical Hardness Relationships with Aromaticity **2015/2016**
Journal of Mathematical Chemistry
47(1) (2010) 487-495; DOI: 10.1007/s10910-009-9585-6
♣ URL: <http://www.springerlink.com/content/f81757qmh225m8v1/> 
34. **PUTZ M.V.** **3.858**^{/34}
On Absolute Aromaticity within Electronegativity and Chemical Hardness **2015/2016**
Reactivity Pictures
MATCH Communications in Mathematical and in Computer Chemistry
64(2) (2010) 391-418
♣ URL: <http://www.pmf.kg.ac.rs/match/content64n2.htm> 
35. **PUTZ M.V.** **3.257**^{/35}
Compactness Aromaticity of Atoms in Molecules **2015/2016**
International Journal of Molecular Sciences
11(4) (2010) 1269-1310; DOI: 10.3390/ijms11041269
(Special Issue: Atoms in Molecules and in Nanostructures (M.V. Putz, editor))
♣ URL: <http://www.mdpi.com/1422-0067/11/4/1269> 

³⁰ <http://www.bioxbio.com/ij/html/J-THEOR-COMPUT-CHEM.html>

³¹ <http://www.bioxbio.com/ij/html/DIG-J-NANOMATER-BIOS.html>

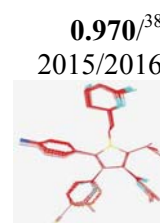
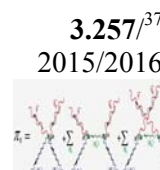
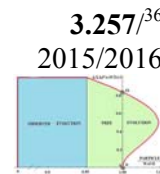
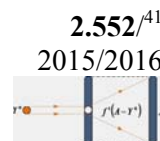
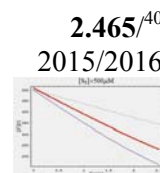
³² <http://chem.ubbcluj.ro/~studiachemia/>

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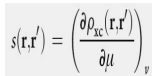
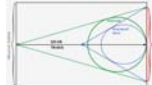
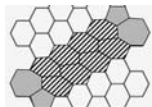
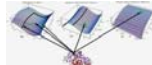
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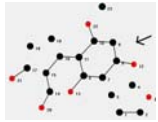
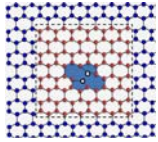
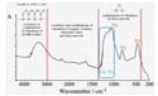
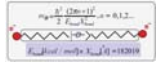
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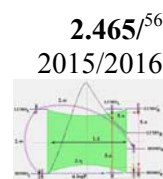
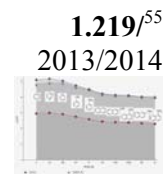
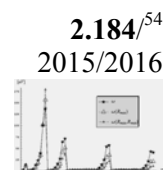
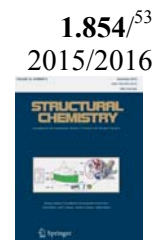
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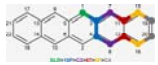
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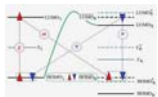
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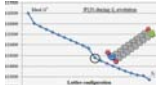
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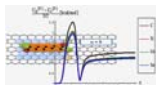
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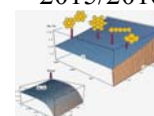
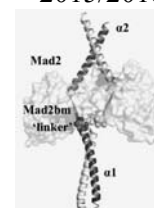
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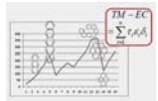
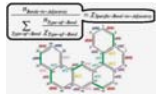
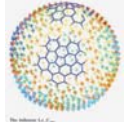
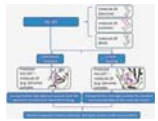
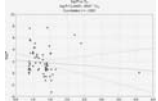


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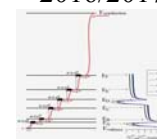
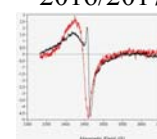
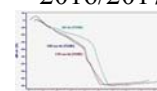
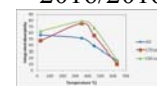
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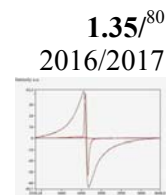
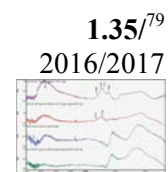
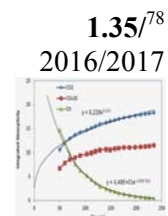
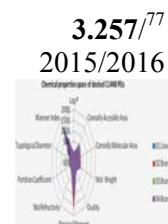
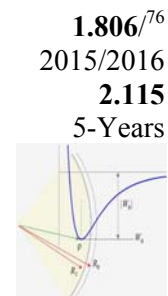
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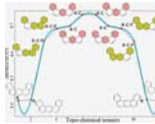
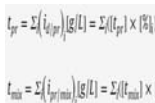
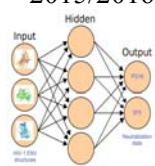
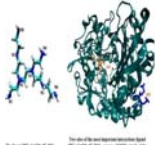
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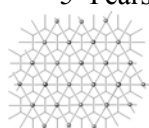
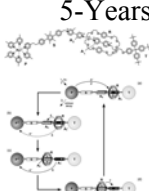
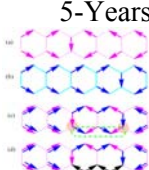
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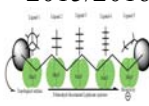
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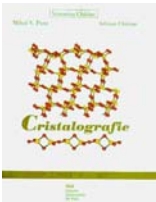
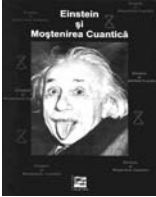
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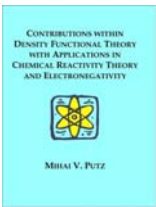
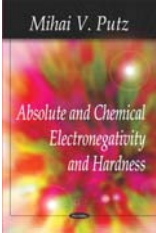
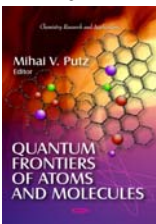
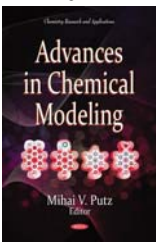
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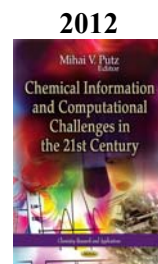
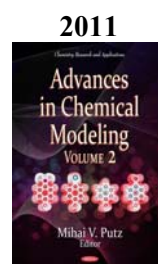
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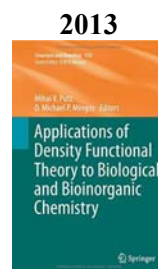
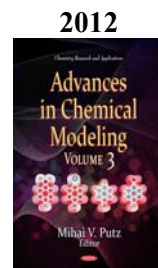
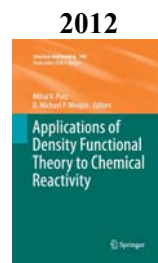
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 ISBN: 978-94-007-1732-9;
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 ♣ URL: <http://www.springer.com/chemistry/physical+chemistry/book/978-94-007-1732-9>
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 ♣ URL: <http://www.appleacademicpress.com/title.php?id=50>
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 ISBN: 978-1-926895-14-7.
 ♣ URL: <http://www.appleacademicpress.com/title.php?id=56>
25. **PUTZ M.V. (Editor)**
CHEMICAL INFORMATION AND COMPUTATIONAL CHALLENGES IN 21ST ~ A Celebration of 2011 International Year of Chemistry ~
 NOVA Science Publishers, Inc., New York, USA
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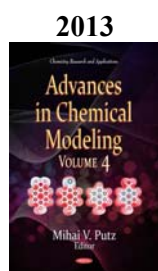


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in "Structure and Bonding" Series Vol. 149,
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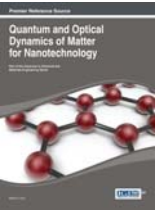
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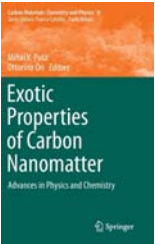
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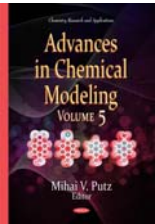
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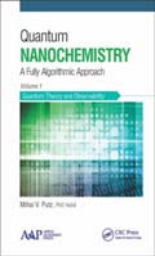
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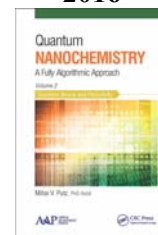

35. **PUTZ M.V.**
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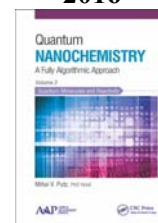


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Vol II. QUANTUM ATOMS AND PERIODICITY
 Apple Academic Press & CRC Press, Toronto-New Jersey, Canada-USA
 pp. 549+index;
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37. **PUTZ M.V.**
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Vol V. QUANTUM STRUCTURE-ACTIVITY RELATIONSHIP (Qu-SAR)
 Apple Academic Press & CRC Press, Toronto-New Jersey, Canada-USA
 pp. 622+index;
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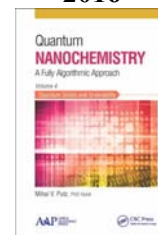
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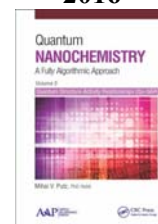
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2016



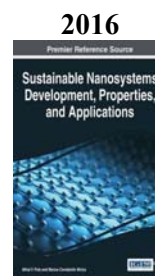
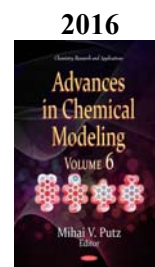
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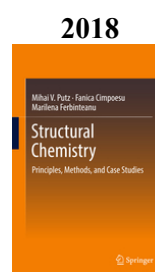


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SUSTAINABLE NANOSYSTEMS DEVELOPMENT, PROPERTIES, AND APPLICATIONS
 IGI Global, Hershey Pasadena, USA
 pp. 794+index; DOI: 10.4018/978-1-5225-0492-4; ISBN13: 9781522504924;
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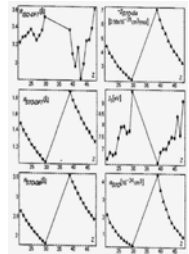
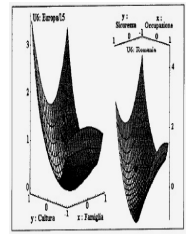
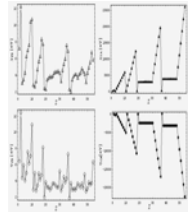


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43. **PUTZ M.V.**
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45.	BELCASTRO M., CHIDO S., KONDAKOVA O., LEOPOLDINI M., MARINO, T., MICHELINI M.C., PUTZ M.V., SICILIA E., TOSCANO M., RUSSO, N. On the Use of Density Functional Theory in the Study of Metal-Ligand Interactions. Some Studied Cases în "METAL-LIGAND INTERACTIONS" Russo, N., Salahub, D.R., Witko, M. (Eds.) NATO Science Series II. Mathematics, Physics and Chemistry – Vol. 116 Kluwer Academic Publishers, Dordrecht, Holland) ISBN: 1-4020-1495-3; pp. 1-20 ♣ URL: http://www.springer.com/chemistry/inorganic/book/978-1-4020-1494-9	2003 
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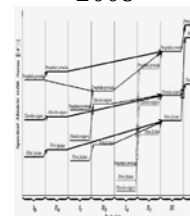
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Quantum and Topological Impact on HMG-CoA Reductase Inhibitors
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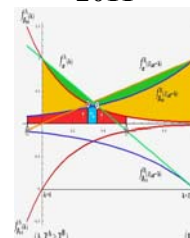
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Designing a Spectral Structure-Activity Ecotoxic-Logistical Battery
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55. **PUTZ M.V.**
Conceptual Density Functional Theory: from Inhomogeneous Electronic Gas to Bose-Einstein Condensates
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Mihai V. Putz (Ed.)
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Hidden Side of Chemical Bond: The Bosonic Condensate
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James C. Taylor (Ed.)
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NOVA Science Publishers, Inc., New York, USA, ISBN: 978-1-61324-018-2,
Chapter 8, pp. 261-298.

2011

$$\begin{aligned} Z &= \int \frac{1}{\Omega} d\Omega \int \frac{1}{\Omega} d\Omega \int \frac{1}{\Omega} d\Omega \\ \eta &= \frac{1}{\Omega} \left(\frac{\partial Z}{\partial \Omega} \right) \\ \eta &= \frac{1}{\Omega} \\ Z &= \int \frac{1}{\Omega} d\Omega \int \frac{1}{\Omega} d\Omega \int \frac{1}{\Omega} d\Omega \\ \eta &= \frac{1}{\Omega} \left(\frac{\partial Z}{\partial \Omega} \right) \\ \eta &= \frac{1}{\Omega} \left(\frac{\partial Z}{\partial \Omega} \right) \end{aligned}$$

2011

$$\begin{aligned} Y_{\text{max}} &= a_1 |a_1\rangle + a_2 |a_2\rangle + \dots + a_n |a_n\rangle + \dots + a_m |a_m\rangle \\ X_1 &= 1 |a_1\rangle + 0 |a_2\rangle + \dots + 0 |a_n\rangle + \dots + 0 |a_m\rangle \\ X_2 &= 0 |a_1\rangle + 1 |a_2\rangle + \dots + 0 |a_n\rangle + \dots + 0 |a_m\rangle \\ X_3 &= 0 |a_1\rangle + 0 |a_2\rangle + \dots + 1 |a_n\rangle + \dots + 0 |a_m\rangle \\ X_m &= 0 |a_1\rangle + 0 |a_2\rangle + \dots + 0 |a_n\rangle + \dots + 1 |a_m\rangle \end{aligned}$$

2011

$$[iE_{\text{KS}}] \psi(r) = - \sum_i E_i \varphi_i(r) \hat{a}_i$$

2011

$$\underbrace{\psi_{BB}(r)}_{\text{BONDONIC}} = \underbrace{c_A \psi_A(r) + c_B \psi_B(r)}_{\text{FERMIONIC SUPERPOSITION}}$$

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Quantum Parabolic Effects of Electronegativity and Chemical Hardness on Carbon π -Systems

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"CARBON BONDING AND STRUCTURES: ADVANCES IN PHYSICS AND CHEMISTRY"

Mihai V. Putz (Ed.)

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ISBN: 978-94-007-1732-9;

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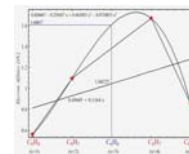
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Logistic versus W-Lambert Information in Modelling Enzyme Kinetics

în

"ADVANCED METHODS AND APPLICATIONS IN CHEMOINFORMATICS: RESEARCH METHODS AND NEW APPLICATIONS"

E.A. Castro, A. K. Haghi (Editors)

IGI Global (formerly Idea Group Inc.), Hershey, PA 17033, USA

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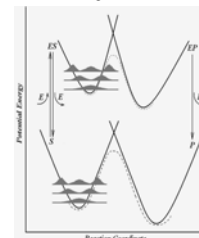
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2011



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Logistic vs. W-Lambert Information in Quantum Modeling of Enzyme Kinetics

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A. K. Haghi (Ed.)

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Chapter 4, pp. 40-59

♣URL: <http://www.igi-global.com/chapter/logistic-lambert-information-quantum-modeling/77068>

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Levels of a Unified Theory of Chemical Interaction
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60. **PUTZ M.V.**
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Turning SPECTRAL-SAR into 3D-QSAR Analysis. Application on H^+K^+ -ATPase Inhibitory Activity
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62. **PUTZ M.V.**
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Mihai V. Putz (Ed.)
NOVA Science Publishers, Inc., New York, USA
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63. **PUTZ M.V., PUTZ A.-M., PITULICE L., CHIRIAC V.**
On Chemical Hardness Assessment of Aromaticity for Some Organic Compound
în
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Mihai V. Putz (Ed.)
NOVA Science Publishers, Inc., New York, USA
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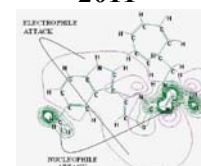
2011

$$\nabla^2 \left[\frac{\sum_{i,j} C_{ij}^{(1)}(x,y)}{\sum_{i,j} C_{ij}^{(2)}(x,y)} \right] = \frac{\sum_{i,j} C_{ij}^{(1)}(x,y)}{\sum_{i,j} C_{ij}^{(2)}(x,y)}$$

2011

$$(\text{curl } \mathbf{E}) \nabla \times \rightarrow \partial / \partial N; \mathbf{H} \rightarrow \mathbf{E}_N$$

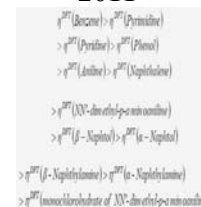
2011



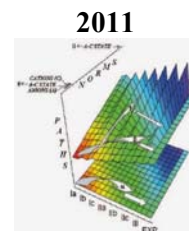
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$$P_B = \frac{F_C}{4\pi r^2} = \frac{\nabla(\Delta C_A^*)}{4\pi r^2}$$

2011



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64. **PUTZ M.V., PUTZ A.-M., OSTAFE V., CHIRIAC A.**
Spectral-SAR Ecotoxicology of Ionic Liquids-Acetylcholine Interaction on *E. Electricus* Species
În "*ADVANCES IN CHEMICAL MODELING. VOLUME 2*"
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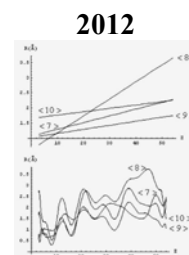
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65. **PUTZ M.V.**
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"*NANOSCIENCE AND ADVANCING COMPUTATIONAL METHODS IN CHEMISTRY: RESEARCH PROGRESS*"
E.A. Castro, A. K. Haghi (Editors)
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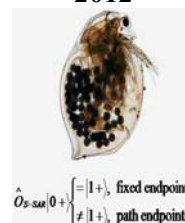
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66. **PUTZ M.V., PUTZ A.M.**
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SPECTRAL-SAR Ecotoxicology of Ionic Liquids: The Daphnia Magna Case
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Mihai V. Putz (Ed.)
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69. **PUTZ M.V.**
On Relationship between Electronic Sharing in Bonding and Electronegativity
Equalization of Atoms in Molecules
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Spectral-SAR Realization of OECD-QSAR Principles
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Compound Formula	Δ	Π	π^*	σ^*	π^*	σ^*
C_6H_6	0.00	0.00	0.00	0.00	0.00	0.00
$\text{C}_6\text{H}_5\text{OH}$	0.01	0.01	0.01	0.01	0.01	0.01
$\text{C}_6\text{H}_5\text{NH}_2$	0.02	0.02	0.02	0.02	0.02	0.02
$\text{C}_6\text{H}_5\text{COOH}$	0.03	0.03	0.03	0.03	0.03	0.03
$\text{C}_6\text{H}_5\text{CHO}$	0.04	0.04	0.04	0.04	0.04	0.04
$\text{C}_6\text{H}_5\text{Cl}$	0.05	0.05	0.05	0.05	0.05	0.05
$\text{C}_6\text{H}_5\text{Br}$	0.06	0.06	0.06	0.06	0.06	0.06
$\text{C}_6\text{H}_5\text{I}$	0.07	0.07	0.07	0.07	0.07	0.07
$\text{C}_6\text{H}_5\text{F}$	0.08	0.08	0.08	0.08	0.08	0.08
$\text{C}_6\text{H}_5\text{NO}_2$	0.09	0.09	0.09	0.09	0.09	0.09
$\text{C}_6\text{H}_5\text{SO}_2\text{Cl}$	0.10	0.10	0.10	0.10	0.10	0.10
$\text{C}_6\text{H}_5\text{SO}_2\text{F}$	0.11	0.11	0.11	0.11	0.11	0.11
$\text{C}_6\text{H}_5\text{SO}_2\text{Br}$	0.12	0.12	0.12	0.12	0.12	0.12
$\text{C}_6\text{H}_5\text{SO}_2\text{I}$	0.13	0.13	0.13	0.13	0.13	0.13
$\text{C}_6\text{H}_5\text{SO}_2\text{NO}_2$	0.14	0.14	0.14	0.14	0.14	0.14
$\text{C}_6\text{H}_5\text{SO}_2\text{ClO}_2$	0.15	0.15	0.15	0.15	0.15	0.15
$\text{C}_6\text{H}_5\text{SO}_2\text{BrO}_2$	0.16	0.16	0.16	0.16	0.16	0.16
$\text{C}_6\text{H}_5\text{SO}_2\text{IO}_2$	0.17	0.17	0.17	0.17	0.17	0.17
$\text{C}_6\text{H}_5\text{SO}_2\text{NO}_2\text{Cl}$	0.18	0.18	0.18	0.18	0.18	0.18
$\text{C}_6\text{H}_5\text{SO}_2\text{NO}_2\text{Br}$	0.19	0.19	0.19	0.19	0.19	0.19
$\text{C}_6\text{H}_5\text{SO}_2\text{NO}_2\text{I}$	0.20	0.20	0.20	0.20	0.20	0.20
$\text{C}_6\text{H}_5\text{SO}_2\text{NO}_2\text{F}$	0.21	0.21	0.21	0.21	0.21	0.21
$\text{C}_6\text{H}_5\text{SO}_2\text{NO}_2\text{ClO}_2$	0.22	0.22	0.22	0.22	0.22	0.22
$\text{C}_6\text{H}_5\text{SO}_2\text{NO}_2\text{BrO}_2$	0.23	0.23	0.23	0.23	0.23	0.23
$\text{C}_6\text{H}_5\text{SO}_2\text{NO}_2\text{IO}_2$	0.24	0.24	0.24	0.24	0.24	0.24
$\text{C}_6\text{H}_5\text{SO}_2\text{NO}_2\text{NO}_2$	0.25	0.25	0.25	0.25	0.25	0.25
$\text{C}_6\text{H}_5\text{SO}_2\text{NO}_2\text{ClO}_2\text{Cl}$	0.26	0.26	0.26	0.26	0.26	0.26
$\text{C}_6\text{H}_5\text{SO}_2\text{NO}_2\text{ClO}_2\text{Br}$	0.27	0.27	0.27	0.27	0.27	0.27
$\text{C}_6\text{H}_5\text{SO}_2\text{NO}_2\text{ClO}_2\text{I}$	0.28	0.28	0.28	0.28	0.28	0.28
$\text{C}_6\text{H}_5\text{SO}_2\text{NO}_2\text{ClO}_2\text{F}$	0.29	0.29	0.29	0.29	0.29	0.29
$\text{C}_6\text{H}_5\text{SO}_2\text{NO}_2\text{ClO}_2\text{ClO}_2$	0.30	0.30	0.30	0.30	0.30	0.30

2012

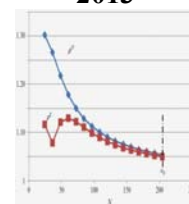


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Element	Symbol	Atomic Number	Atomic Weight	Electronegativity	Ionization Potential	Electron Affinity
Hydrogen	H	1	1.008	2.20	13.12 eV	72.8 kJ/mol
Helium	He	2	4.003	0.00	23.72 eV	48.4 kJ/mol
Lithium	Li	3	6.941	0.98	5.39 eV	60 kJ/mol
Boron	B	5	10.81	2.04	8.01 eV	267 kJ/mol
Carbon	C	6	12.01	2.55	11.41 eV	121 kJ/mol
Nitrogen	N	7	14.01	3.04	14.53 eV	140 kJ/mol
Oxygen	O	8	16.00	3.44	13.61 eV	141 kJ/mol
Fluorine	F	9	18.99	3.98	16.81 eV	328 kJ/mol
Neon	Ne	10	20.18	0.00	20.81 eV	1199 kJ/mol
Sodium	Na	11	22.99	0.93	5.14 eV	55 kJ/mol
Magnesium	Mg	12	24.31	1.31	7.38 eV	73.8 kJ/mol
Aluminum	Al	13	26.98	1.61	5.78 eV	42 kJ/mol
Silicon	Si	14	28.09	1.90	8.45 eV	111 kJ/mol
Phosphorus	P	15	30.97	2.19	10.49 eV	72 kJ/mol
Sulfur	S	16	32.07	2.58	12.07 eV	200 kJ/mol
Chlorine	Cl	17	35.45	3.16	12.51 eV	349 kJ/mol
Argon	Ar	18	39.95	0.00	15.21 eV	1521 kJ/mol
Potassium	K	19	39.10	0.82	4.19 eV	41.8 kJ/mol
Calcium	Ca	20	40.08	1.00	6.11 eV	59 kJ/mol
Scandium	Sc	21	44.96	1.36	6.56 eV	38 kJ/mol
Titanium	Ti	22	47.88	1.54	7.92 eV	78 kJ/mol
Vanadium	V	23	50.94	1.63	8.51 eV	122 kJ/mol
Chromium	Cr	24	51.99	1.66	7.76 eV	141 kJ/mol
Manganese	Mn	25	54.94	1.55	7.43 eV	150 kJ/mol
Iron	Fe	26	55.85	1.83	7.64 eV	157 kJ/mol
Cobalt	Co	27	58.93	1.88	7.86 eV	164 kJ/mol
Nickel	Ni	28	58.69	1.91	7.73 eV	161 kJ/mol
Copper	Cu	29	63.55	1.90	7.72 eV	168 kJ/mol
Zinc	Zn	30	65.38	1.65	7.86 eV	173 kJ/mol
Gallium	Ga	31	69.72	1.81	7.82 eV	173 kJ/mol
Germanium	Ge	32	72.64	2.01	7.86 eV	173 kJ/mol
Arsenic	As	33	74.92	2.02	8.15 eV	173 kJ/mol
Selenium	Se	34	78.96	2.55	8.14 eV	173 kJ/mol
Bromine	Br	35	79.90	2.96	8.01 eV	173 kJ/mol
Krypton	Kr	36	83.80	0.00	11.00 eV	1100 kJ/mol
Rubidium	Rb	37	85.47	0.82	4.18 eV	41.8 kJ/mol
Strontium	Sr	38	87.62	1.00	6.11 eV	59 kJ/mol
Yttrium	Y	39	88.91	1.22	6.30 eV	38 kJ/mol
Zirconium	Zr	40	91.22	1.33	7.44 eV	78 kJ/mol
Niobium	Nb	41	92.91	1.45	7.43 eV	78 kJ/mol
Molybdenum	Mo	42	95.94	1.68	7.38 eV	78 kJ/mol
Technetium	Tc	43	98.01	1.90	7.72 eV	78 kJ/mol
Ruthenium	Ru	44	101.07	1.88	7.73 eV	78 kJ/mol
Rhodium	Rh	45	102.91	1.88	7.84 eV	78 kJ/mol
Palladium	Pd	46	106.42	1.88	7.73 eV	78 kJ/mol
Silver	Ag	47	107.87	1.93	7.84 eV	78 kJ/mol
Cadmium	Cd	48	112.41	1.69	7.84 eV	78 kJ/mol
Indium	In	49	114.82	1.78	7.84 eV	78 kJ/mol
Sn	Sn	50	118.71	1.82	7.84 eV	78 kJ/mol
Antimony	Sb	51	121.76	1.82	8.14 eV	78 kJ/mol
Tellurium	Te	52	127.60	2.10	8.14 eV	78 kJ/mol
Iodine	I	53	126.91	2.50	8.14 eV	78 kJ/mol
Xenon	Xe	54	131.29	0.00	11.00 eV	1100 kJ/mol
Cesium	Cs	55	132.91	0.82	4.18 eV	41.8 kJ/mol
Barium	Ba	56	137.33	1.00	6.11 eV	59 kJ/mol
Lanthanum	La	57	138.91	1.10	6.30 eV	38 kJ/mol
Cerium	Ce	58	140.12	1.10	6.30 eV	38 kJ/mol
Praseodymium	Pr	59	140.91	1.13	6.30 eV	38 kJ/mol
Neodymium	Nd	60	144.24	1.14	6.30 eV	38 kJ/mol
Europium	Eu	63	151.96	1.10	6.30 eV	38 kJ/mol
Gadolinium	Gd	64	157.25	1.10	6.30 eV	38 kJ/mol
Terbium	Tb	65	158.93	1.10	6.30 eV	38 kJ/mol
Dysprosium	Dy	66	162.50	1.10	6.30 eV	38 kJ/mol
Ytterbium	Yb	70	173.05	1.10	6.30 eV	38 kJ/mol
Lutetium	Lu	71	174.97	1.10	6.30 eV	38 kJ/mol
Hafnium	Hf	72	178.49	1.33	7.44 eV	78 kJ/mol
Tantalum	Ta	73	180.95	1.45	7.43 eV	78 kJ/mol
Tungsten	W	74	183.85	1.68	7.38 eV	78 kJ/mol
Rhenium	Re	75	186.21	1.90	7.72 eV	78 kJ/mol
Osmium	Os	76	190.23	1.88	7.73 eV	78 kJ/mol
Iridium	Ir	77	192.22	1.88	7.84 eV	78 kJ/mol
Platinum	Pt	78	195.08	1.88	7.73 eV	78 kJ/mol
Gold	Au	79	196.97	1.93	7.84 eV	78 kJ/mol
Mercury	Hg	80	200.59	1.69	7.84 eV	78 kJ/mol
Thallium	Tl	81	204.38	1.78	7.84 eV	78 kJ/mol
Lead	Pb	82	207.2	1.82	7.84 eV	78 kJ/mol
Bismuth	Bi	83	208.98	1.82	8.14 eV	78 kJ/mol
Polonium	Po	84	209	2.10	8.14 eV	78 kJ/mol
Astatine	At	85	210	2.50	8.14 eV	78 kJ/mol
Radon	Rn	86	222	0.00	11.00 eV	1100 kJ/mol
Francium	Fr	87	223	0.82	4.18 eV	41.8 kJ/mol
Radium	Ra	88	226	1.00	6.11 eV	59 kJ/mol
Actinium	Ac	89	227	1.10	6.30 eV	38 kJ/mol
Thorium	Th	90	232.04	1.10	6.30 eV	38 kJ/mol
Protactinium	Pa	91	231.04	1.10	6.30 eV	38 kJ/mol
Uranium	U	92	238.03	1.10	6.30 eV	38 kJ/mol
Np	Np	93	237.05	1.10	6.30 eV	38 kJ/mol
Pu	Pu	94	244.06	1.10	6.30 eV	38 kJ/mol
Am	Am	95	243.06	1.10	6.30 eV	38 kJ/mol
Cm	Cm	96	247.07	1.10	6.30 eV	38 kJ/mol
Bk	Bk	97	247.07	1.10	6.30 eV	38 kJ/mol
Cf	Cf	98	251.08	1.10	6.30 eV	38 kJ/mol
Es	Es	99	252.08	1.10	6.30 eV	38 kJ/mol
Fm	Fm	100	257.10	1.10	6.30 eV	38 kJ/mol
Mendelevium	Md	101	258.10	1.10	6.30 eV	38 kJ/mol
Nobelium	No	102	259.10	1.10	6.30 eV	38 kJ/mol
Lr	Lr	103	262.11	1.10	6.30 eV	38 kJ/mol
Rutherfordium	Rf	104	261.11	1.33	7.44 eV	78 kJ/mol
Dubnium	Db	105	262.11	1.45	7.43 eV	78 kJ/mol
Seaborgium	Sg	106	266.12	1.68	7.38 eV	78 kJ/mol
Berkelium	Bk	107	267.12	1.90	7.72 eV	78 kJ/mol
Californium	Cf	108	271.13	1.88	7.73 eV	78 kJ/mol
Einsteinium	Es	109	272.13	1.88	7.84 eV	78 kJ/mol
Fermium	Fm	110	277.14	1.88	7.73 eV	78 kJ/mol
Mendelevium	Md	111	278.14	1.88	7.84 eV	78 kJ/mol
Nobelium	No	112	289.15	1.88	7.73 eV	78 kJ/mol
Lr	Lr	113	290.15	1.93	7.84 eV	78 kJ/mol
Uut	Uut	114	289.15	1.69	7.84 eV	78 kJ/mol
Uuq	Uuq	115	288.15	1.78	7.84 eV	78 kJ/mol
Uub	Uub	116	287.15	1.82	7.84 eV	78 kJ/mol
Uuh	Uuh	117	288.15	2.10	8.14 eV	78 kJ/mol
Uus	Uus	118	289.15	2.50	8.14 eV	78 kJ/mol
Uuo	Uuo	119	293.15	0.00	11.00 eV	1100 kJ/mol
Uut	Uut	120	294.15	0.82	4.18 eV	41.8 kJ/mol
Uuq	Uuq	121	295.15	1.00	6.11 eV	59 kJ/mol
Uub	Uub	122	296.15	1.10	6.30 eV	38 kJ/mol
Uuh	Uuh	123	297.15	1.10	6.30 eV	38 kJ/mol
Uus	Uus	124	299.15	1.10	6.30 eV	38 kJ/mol
Uuo	Uuo	125	301.15	1.10	6.30 eV	38 kJ/mol
Uut	Uut	126	303.15	1.10	6.30 eV	38 kJ/mol
Uuq	Uuq	127	305.15	1.10	6.30 eV	38 k

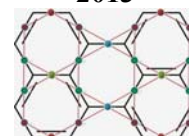
75. **PUTZ M.V.**, DE CORATO M., BENEDEK G., SEDLAR J., GRAOVAC A., ORI O.
Topological Invariants of Moebius-Like Graphenic Nanostructures
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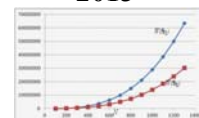
77. **PUTZ M.V.**
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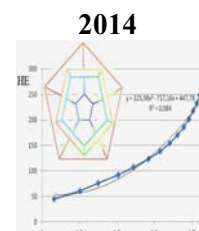
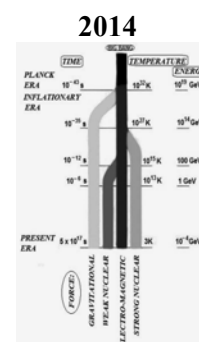
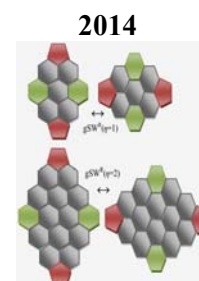
$$\left(-\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(\mathbf{r}) + g|\psi(\mathbf{r})|^2 \right) \psi(\mathbf{r}) = \mu \psi(\mathbf{r})$$

78. DE CORATO M., BENEDEK G., ORI O., **PUTZ M.V.**
Topological Study of Schwarzitic Junctions in 1D Lattices
în
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Mihai V. Putz (Ed.)
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Modeling Chlorinated Polycyclic Aromatic Hydrocarbons (Cl-PAH) Eco- and Toxicology by QSAR-OECD ToolBox Facility
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♣ URL: https://www.novapublishers.com/catalog/product_info.php?products_id=43018
80. ORI O., **PUTZ M.V.**, GUTMAN I., SCHWERDTFEGER P.
Generalized Stone-Wales Transformations for Fullerene Graphs Derived from Berge's Switching Theorem
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"ANTE GRAOVAC – LIFE AND WORKS"
Gutman I., Pokrić B., Vukičević D. (Eds.),
MATHEMATICAL CHEMISTRY MONOGRAPHS, No. 16
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81. **PUTZ M.V.**
Nanouniverse Expanding Macrouniverse: From Elementary Particles to Dark Matter and Energy
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Mihai V. Putz (Ed.)
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82. KOOREPAZAN–MOFTAKHAR F., ASHRAFI A.R., ORI O., **PUTZ M.V.**
Sphericity of Some Classes of Fullerenes Measured by Topology
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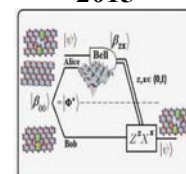


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Geometry and Topology of Nanotubes and Nanotori
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♣URL: <http://www.springer.com/chemistry/theoretical+and+computational+chemistry/book/978-94-017-9566-1>
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Bondonic Chemistry: Physical Origins and Entanglement Prospects
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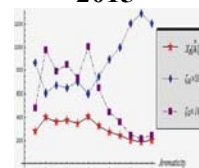
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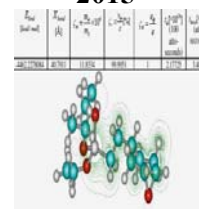
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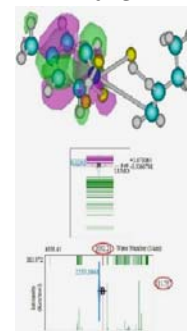
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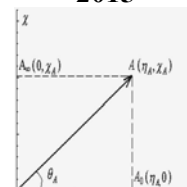
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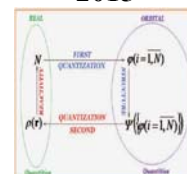
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$$\begin{aligned}
 |Y\rangle &= a_0|X_0\rangle + a_1|X_1\rangle + \dots + a_M|X_M\rangle \\
 |X_0\rangle &= S^{(-1)}|X_0\rangle + 0|X_1\rangle + \dots + 0|X_M\rangle \\
 |X_1\rangle &= 0|X_0\rangle + S^{(-1/2)}|X_1\rangle + \dots + 0|X_M\rangle \\
 &\vdots \\
 |X_M\rangle &= 0|X_0\rangle + 0|X_1\rangle + \dots + S^{(-1/2)}|X_M\rangle
 \end{aligned}$$

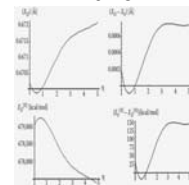
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 Bondonic Electronic Properties of 2D Graphenic Lattices with Structural Defects
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 Mahmood Aliofkhazraei, Nasar Ali, William I. Milne, Cengiz S. Ozkan,
 Stanislaw Mitura, Juana L. Gervasoni (Eds.)
 CRC Pres, Taylor & Francis Group, Boca Raton, Florida, USA
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 ♣URL: <https://www.crcpress.com/Graphene-Science-Handbook-Electrical-and-Optical-Properties/Aliofkhazraei-Ali-Milne-Ozkan-Mitura-Gervasoni/p/book/9781466591318>

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DISTANCES, SYMMETRY AND TOPOLOGY IN CARBON NANOMATERIALS
 Ali Reza Ashrafi; Mircea V. Diudea (Eds.)
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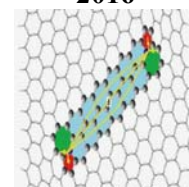
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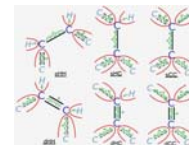
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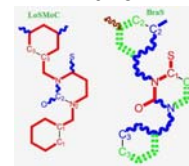


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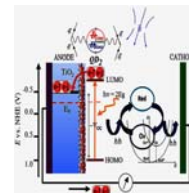


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Mihai V. Putz, Marius Constantin Mirica (Eds.)
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Sustainable Design of Photovoltaics: Devices and Quantum Information
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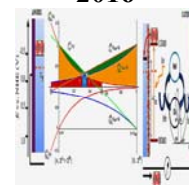
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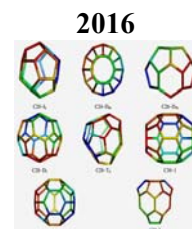
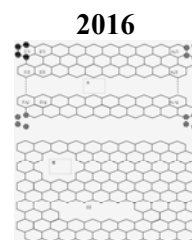
$$f_{\text{ph}}^{-1} = 18.8177 \times 10^9 \times \Delta \tilde{\nu}_{\text{PRR}} [\text{cm}^{-1}]$$

$$I_n = 2\phi f = 2\phi [18.8177 \times 10^9 \times \Delta \tilde{\nu}_{\text{PRR}}] [\text{cm}^{-1}]$$

$$V_n = \frac{h}{2e} f = \frac{h}{2e} [18.8177 \times 10^9 \times \Delta \tilde{\nu}_{\text{PRR}}] [\text{cm}^{-1}]$$

$$I_{\text{sc}} \times V_{\text{oc}} = \frac{2\phi h}{1Q} [18.8177 \times 10^9 \times \Delta \tilde{\nu}_{\text{PRR}}] [\text{cm}^{-1}]^2$$

99. ORI O., CATALDO F., **PUTZ M.V.**
Entropy of Nanostructures: Topological Effects on Schottky Vacancies
Concentration in Graphenic Bidimensional HC(N) Lattices
în
SUSTAINABLE NANOSYSTEMS DEVELOPMENT, PROPERTIES, AND APPLICATIONS
Mihai V. Putz, Marius Constantin Mirica (Eds.)
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