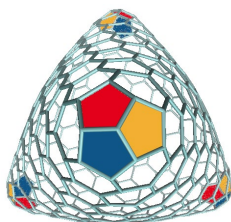




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**Timișoara    Ianuarie 2023**

## LISTA DE LUCRĂRI

### **SYNOPSIS:**


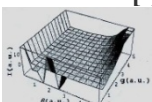

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**(i) TEZE DE DOCTORAT ȘI ABILITARE**

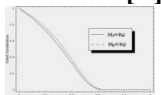
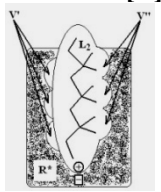
Informații Teza de Doctorat	Data Susținerii
<p><b>PUTZ M.V.</b>  <i>CONTRIBUȚII LA TEORIA FUNCȚIONALEI DENSITATE CU APLICAȚII ÎN TEORIA REACTIVITĂȚII CHIMICE ȘI A ELECTRONEGATIVITĂȚII</i>  <b>Universitatea de Vest din Timișoara</b>                      publicată ulterior în limba Engleză  <i>Contributions within Density Functional Theory with Applications to Chemical Reactivity Theory and Electronegativity</i>                      în versiune extinsă la                      Disertation. Com, Parkland, Florida, USA (2003) pag. 180;                      ISBN: 1-58112-184-9;                      ♣URL: <a href="http://dissertation.com/books/1581121849">http://dissertation.com/books/1581121849</a></p>	<p><b>2002</b>  <b>15 Martie</b>  <b>DOCTORAT</b>  <b>CHIMIE</b></p>
<p><b>PUTZ M.V.</b>  <i>DINAMICA STRATEGICĂ A POTENȚIALULUI DE CERCETARE-DEZVOLTARE-INOVARĂ ÎN (META)CLUSTERE NANOTEHNOLOGICE</i>  <b>Universitatea de Vest din Timișoara</b>                      publicată ulterior în limba Engleză, în co-autorat extins (cu Prof. Ioan I. Petrișor)  <i>The Code Of Strategic Management</i>                      la                      Apple Academic Press USA&amp; Canada (2022/2023) pag. 250;                      ISBN:;                      ♣URL:</p>	<p><b>2021</b>  <b>24Septembrie</b>  <b>DOCTORAT</b>  <b>MANAGEMENT</b></p>

Informații Teza de Abilitare	Data Susținerii
<p><b>PUTZ M.V.</b>  <i>CHEMICAL ORTHOGONAL SPACES OF ATOMS AND MOLECULES</i>  <b>Universitatea Babeș-Bolyai din Cluj-Napoca</b>                      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: <a href="https://match.pmf.kg.ac.rs/mcm14.html">https://match.pmf.kg.ac.rs/mcm14.html</a></p>	<p><b>2013</b>  <b>20 Martie</b>  <b>ABILITARE</b>  <b>CHIMIE</b></p>

**(ii) ARTICOLE ISI THOMPSON REUTERS**

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

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

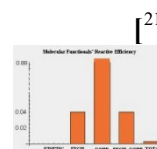
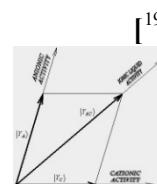
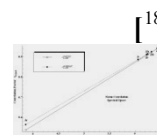
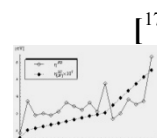
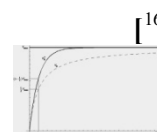
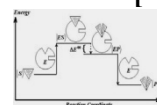
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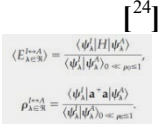
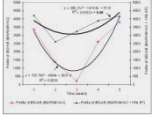
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31. **GHIJU S., PUTZ M.V. (\*), CHIRIAC A.**  
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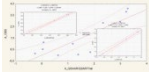
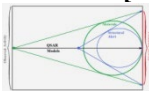
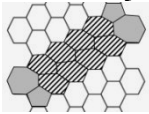
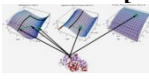
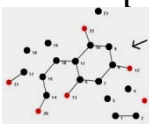
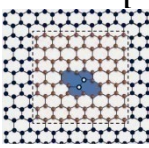
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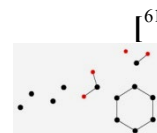
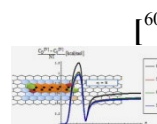
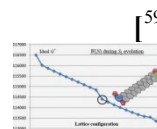
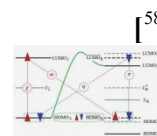
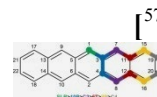
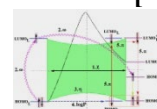
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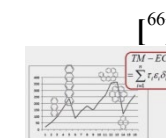
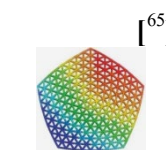
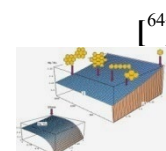
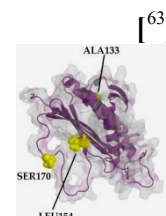
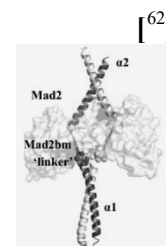
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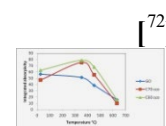
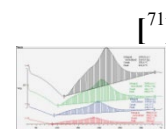
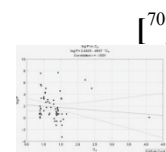
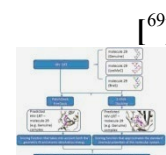
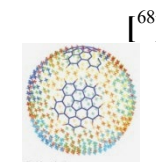
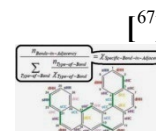
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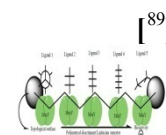
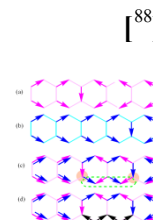
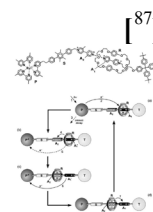
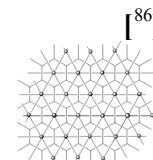
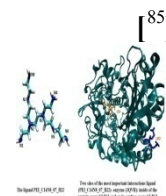
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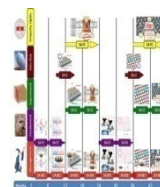


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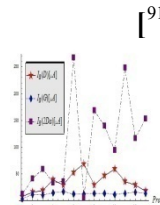


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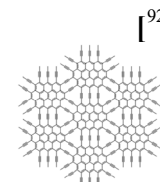


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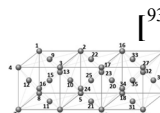


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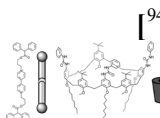


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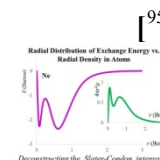


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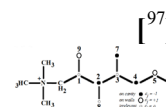
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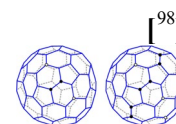
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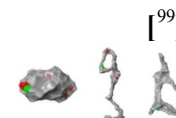
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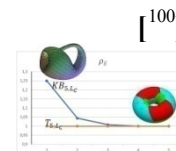
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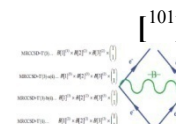
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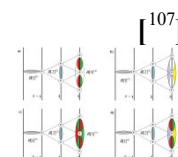
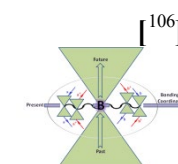
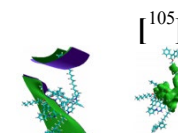
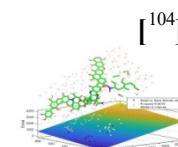
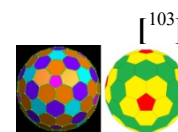
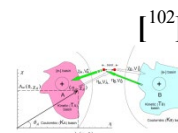
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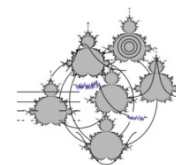
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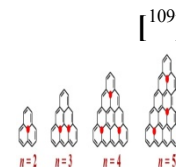
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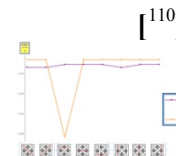


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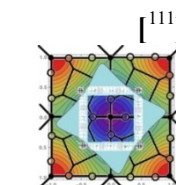
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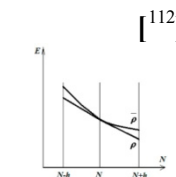
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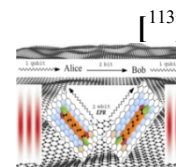
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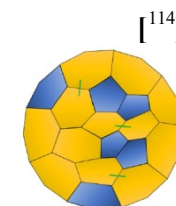
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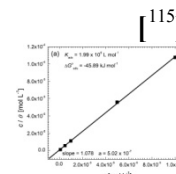
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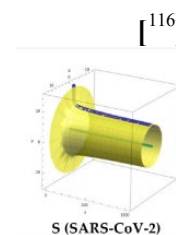
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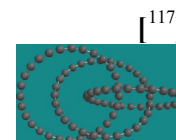
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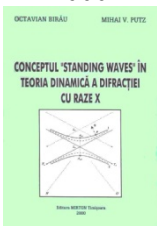
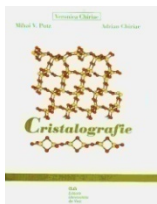
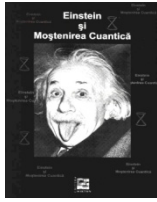

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2006



2006



2007



2008



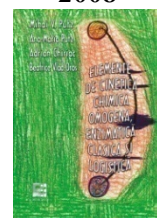
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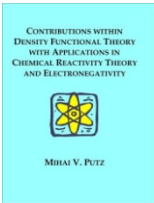
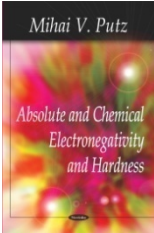
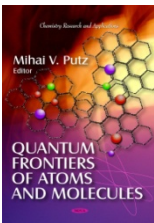
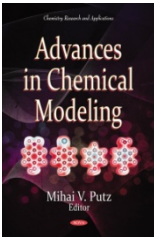
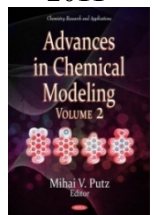
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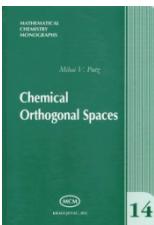


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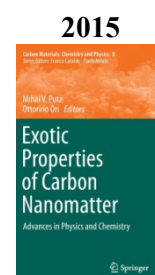
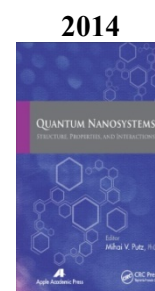
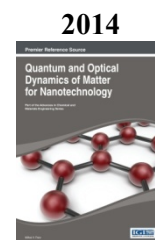
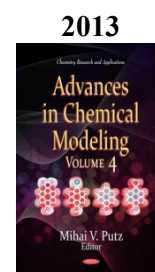
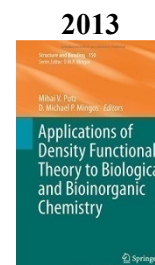
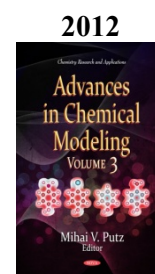


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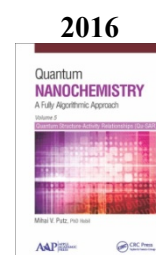
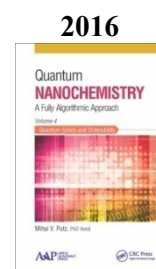
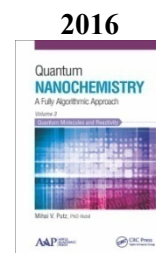
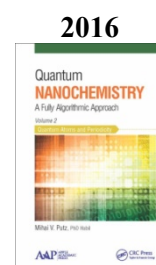
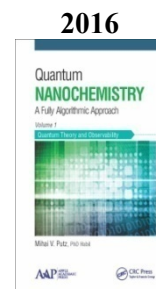
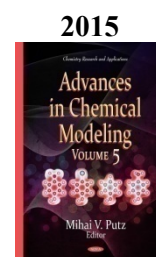
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- 2012
27. **PUTZ M.V., MINGOS D.M.P.** (Editors)  
*APPLICATIONS OF DENSITY FUNCTIONAL THEORY TO CHEMICAL REACTIVITY*  
 in “Structure and Bonding” Series Vol. 149,  
 Springer Verlag, Heidelberg-Berlin, Germany  
 pp. 189;  
 ISBN (Hardcover): 978-3-642-32752-0  
 ♣URL: <http://www.springer.com/chemistry/inorganic+chemistry/book/978-3-642-32752-0>
- 
- 2012

28. **PUTZ M.V.** (Editor)  
*ADVANCES IN CHEMICAL MODELING. VOLUME 3*  
 NOVA Science Publishers, Inc., New York, USA  
 pp. 494;  
 ISBN: 978-1-62257-110-9  
 ♣URL: [https://www.novapublishers.com/catalog/product\\_info.php?products\\_id=34573](https://www.novapublishers.com/catalog/product_info.php?products_id=34573)
29. **PUTZ M.V., MINGOS D.M.P.** (Editors)  
*APPLICATIONS OF DENSITY FUNCTIONAL THEORY TO BIOLOGICAL AND BIOINORGANIC CHEMISTRY*  
 in "Structure and Bonding" Series Vol. 150,  
 Springer Verlag, Heidelberg-Berlin, Germany  
 pp. 248;  
 ISBN (Hardcover): 978-3-642-32749-0  
 ♣URL: <http://www.springer.com/chemistry/inorganic+chemistry/book/978-3-642-32749-0>
30. **PUTZ M.V.** (Editor)  
*ADVANCES IN CHEMICAL MODELING. VOLUME 4*  
 NOVA Science Publishers, Inc., New York, USA  
 pp. 572;  
 ISBN: 978-1-62808-186-2  
 ♣URL: [https://www.novapublishers.com/catalog/product\\_info.php?products\\_id=43018](https://www.novapublishers.com/catalog/product_info.php?products_id=43018)
31. **PUTZ M.V.**  
*QUANTUM AND OPTICAL DYNAMICS OF MATTER FOR NANOTECHNOLOGY*  
 IGI Global, Hershey Pasadena, USA  
 pp. 527; DOI: 10.4018/978-1-4666-4687-2; ISBN13: 9781466646872;  
 ISBN10: 146664687X; EISBN13: 9781466646889  
 ♣URL: <http://www.igi-global.com/book/quantum-optical-dynamics-matter-nanotechnology/77401>
32. **PUTZ M.V.** (Editor)  
*QUANTUM NANOSYSTEMS. STRUCTURE, PROPERTIES AND INTERACTIONS*  
 Apple Academic Press & CRC Press, Toronto-New Jersey, Canada-USA  
 pp. 504;  
 ISBN: 978-1-926895-90-1  
 ♣URL: <http://www.appleacademicpress.com/title.php?id=9781926895901>
33. **PUTZ M.V., ORI O.** (Editori)  
*EXOTIC PROPERTIES OF CARBON NANOMATTER: ADVANCES IN PHYSICS AND CHEMISTRY*  
 Springer Verlag, Dordrecht, NL,  
 pp. 398;  
 ISBN: 978-94-017-9566-1;  
*Book included as Vol.8 in the SERIES „CARBON MATERIALS: CHEMISTRY AND PHYSICS” (Series Editors: Franco Cataldo, Paolo Milani), Series ISSN: 1875-0745*



♣URL:<http://www.springer.com/chemistry/theoretical+and+computational+chemistry/book/978-94-017-9566-1>

34. **PUTZ M.V.** (Editor)  
*ADVANCES IN CHEMICAL MODELING. VOLUME 5*  
 NOVA Science Publishers, Inc., New York, USA  
 pp. 523;  
 ISBN: 978-1-63482-310-4  
 ♣URL: [https://www.novapublishers.com/catalog/product\\_info.php?products\\_id=53938](https://www.novapublishers.com/catalog/product_info.php?products_id=53938)
35. **PUTZ M.V.**  
*QUANTUM NANOCHEMISTRY. A Fully Integrated Approach: Vol I. QUANTUM THEORY AND OBSERVABILITY*  
 Apple Academic Press & CRC Press, Toronto-New Jersey, Canada-USA  
 pp. 651+index;  
 ISBN: 978-1-771881-33-3  
 ♣URL:<http://www.appleacademicpress.com/title.php?id=9781771881333>
36. **PUTZ M.V.**  
*QUANTUM NANOCHEMISTRY. A Fully Integrated Approach: Vol II. QUANTUM ATOMS AND PERIODICITY*  
 Apple Academic Press & CRC Press, Toronto-New Jersey, Canada-USA  
 pp. 549+index;  
 ISBN: 978-1-771881-34-0  
 ♣URL: <http://www.appleacademicpress.com/title.php?id=9781771881340>
37. **PUTZ M.V.**  
*QUANTUM NANOCHEMISTRY. A Fully Integrated Approach: Vol III. QUANTUM MOLECULES AND REACTIVITY*  
 Apple Academic Press & CRC Press, Toronto-New Jersey, Canada-USA  
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 ISBN: 978-1-771881-35-7  
 ♣URL: <http://www.appleacademicpress.com/title.php?id=9781771881357>
38. **PUTZ M.V.**  
*QUANTUM NANOCHEMISTRY. A Fully Integrated Approach: Vol IV. QUANTUM SOLIDS AND ORDERABILITY*  
 Apple Academic Press & CRC Press, Toronto-New Jersey, Canada-USA  
 pp. 686+index;  
 ISBN: 978-1-771881-36-4  
 ♣URL: <http://www.appleacademicpress.com/title.php?id=9781771881364>
39. **PUTZ M.V.**  
*QUANTUM NANOCHEMISTRY. A Fully Integrated Approach: Vol V. QUANTUM STRUCTURE-ACTIVITY RELATIONSHIP (Qu-SAR)*  
 Apple Academic Press & CRC Press, Toronto-New Jersey, Canada-USA  
 pp. 622+index;  
 ISBN: 978-1-771881-37-1  
 ♣URL: <http://www.appleacademicpress.com/title.php?id=9781771881371>



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Vol V. *QUANTUM STRUCTURE-ACTIVITY RELATIONSHIP (Qu-SAR)*

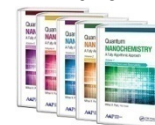
Apple Academic Press & CRC Press, Toronto-New Jersey, Canada-USA

pp. 3086+index;

ISBN: 978-1-771881-38-8

♣ URL: <http://www.appleacademicpress.com/title.php?id=9781771881388>

**2016**



40. **PUTZ M.V.** (Editor)

*ADVANCES IN CHEMICAL MODELING. VOLUME 6*

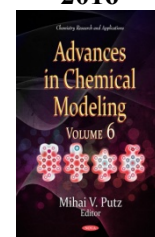
NOVA Science Publishers, Inc., New York, USA

pp. 640;

ISBN: 978-1-63485-030-8

♣ URL: <https://novapublishers.com/shop/advances-in-chemical-modeling-volume-6/>

**2016**



41. **PUTZ M.V.**, MIRICĂ M.C. (Editori)

*SUSTAINABLE NANOSYSTEMS DEVELOPMENT, PROPERTIES, AND APPLICATIONS*

IGI Global, Hershey Pasadena, USA

pp. 794+index; DOI: 10.4018/978-1-5225-0492-4; ISBN13: 9781522504924;

ISBN10: 1522504923; EISBN13: 9781522504931

♣ URL: <http://www.igi-global.com/book/sustainable-nanosystems-development-properties-applications/147016>

**2016**



42. **PUTZ M.V.**, CIMPOEȘU F., FERBINȚEANU M.

*STRUCTURAL CHEMISTRY : PRINCIPLES, METHODS, AND CASE STUDIES ON THE MOLECULAR AND NANOSCALE*

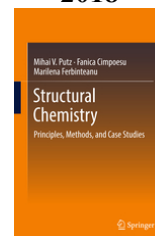
Springer Verlag, Dordrecht, NL,

E-Book ISBN: 978-3-319-55875-2; Hard-Book ISBN: 978-3-319-55873-8;

pp. ~ 800+index;

♣ URL: <http://www.springer.com/gp/book/9783319558738>

**2018**



43. **PUTZ M.V.**

*THE CUBE OF STRATEGIC MANAGEMENT. THE DISTINCTIVE ADVANTAGE OF ORGANIZATIONS*

Apple Academic Press & CRC Press, Toronto-New Jersey, Canada-USA

pp. 306+index;

ISBN: 978-1-771887-75-5

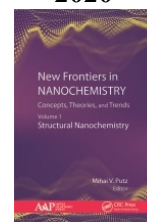
♣ URL: <http://www.appleacademicpress.com/the-cube-of-strategic-management-the-distinctive-advantage-of-organizations/9781771887755>

**2019**

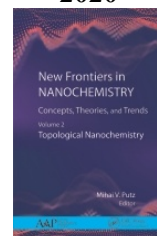


44. **PUTZ M.V.** (Editor)  
NEW FRONTIERS IN NANOCHEMISTRY: CONCEPTS, THEORIES, AND TRENDS, VOLUME 1: STRUCTURAL NANOCHEMISTRY  
Apple Academic Press & CRC Press, Toronto-New Jersey, Canada-USA  
pp. 526+index;  
ISBN: 978-1-771887-77-9  
♣URL: <http://www.appleacademicpress.com/new-frontiers-in-nanochemistry-concepts-theories-and-trends-volume-1-structural-nanochemistry-/9781771887779>
45. **PUTZ M.V.** (Editor)  
NEW FRONTIERS IN NANOCHEMISTRY: CONCEPTS, THEORIES, AND TRENDS, VOLUME 2: TOPOLOGICAL NANOCHEMISTRY  
Apple Academic Press & CRC Press, Toronto-New Jersey, Canada-USA  
pp. 606+index;  
ISBN: 978-1-771887-78-6  
♣URL: <http://www.appleacademicpress.com/new-frontiers-in-nanochemistry-concepts-theories-and-trends-volume-2-topological-nanochemistry-/9781771887786>
46. **PUTZ M.V.** (Editor)  
NEW FRONTIERS IN NANOCHEMISTRY: CONCEPTS, THEORIES, AND TRENDS, VOLUME 3: SUSTAINABLE NANOCHEMISTRY  
Apple Academic Press & CRC Press, Toronto-New Jersey, Canada-USA  
pp. 504+index;  
ISBN: 978-1-771887-79-3  
♣URL: <http://www.appleacademicpress.com/new-frontiers-in-nanochemistry-concepts-theories-and-trends-volume-3-sustainable-nanochemistry-/9781771887793>

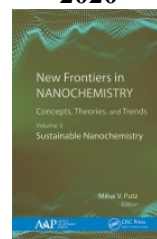
2020



2020



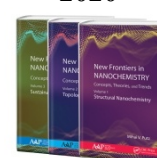
2020



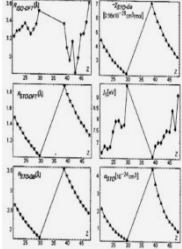
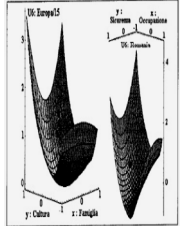
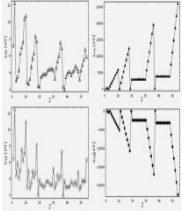
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Apple Academic Press & CRC Press, Toronto-New Jersey, Canada-USA  
pp. 1479+index;  
ISBN: 978-1-771887-80-9  
♣URL: <http://www.appleacademicpress.com/new-frontiers-in-nanochemistry-concepts-theories-and-trends-3-volume-set-volume-1-structural-nanochemistrybrvolume-2-topological-nanochemistrybrvolume-3-sustainable-nanochemistry/9781771887809>

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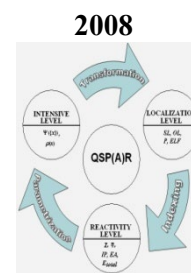


**(v) CAPITOLE ÎN CĂRȚI**

Nr.	Informatii Capitol de Carte	An Apariție
47.	<p>BELCASTRO M., CHIODO S., KONDAKOVA O., LEOPOLDINI M., MARINO, T., MICHELINI M.C., <b>PUTZ M.V.</b>, SICILIA E., TOSCANO M., RUSSO, N.</p> <p>On the Use of Density Functional Theory in the Study of Metal-Ligand Interactions. Some Studied Casesîn "<i>METAL-LIGAND INTERACTIONS</i>"</p> <p>Russo, N., Salahub, D.R., Witko, M. (Eds.)</p> <p>NATO Science Series II. Mathematics, Physics and Chemistry – Vol. 116</p> <p>Kluwer Academic Publishers, Dordrecht, Holland)</p> <p>ISBN: 1-4020-1495-3; pp. 1-20</p> <p>♣URL: <a href="http://www.springer.com/chemistry/inorganic/book/978-1-4020-1494-9">http://www.springer.com/chemistry/inorganic/book/978-1-4020-1494-9</a></p>	<p><b>2003</b></p> 
48.	<p><b>PUTZ M.V.</b></p> <p>"Devianza, Minori e Teoria delle Catastrofi: un Approach Integrato e le Sue Applicazioni"</p> <p>în</p> <p>"<i>CATASTROFI ESISTENZIALI-ANATOMIA DEL DISAGIO GIOVANILE</i>"</p> <p>editată de Silvana Palazzo</p> <p>cu un o Prefață de Giovanni Latorre (Rectorul Universității din Calabria), Periferia Editori, Cosenza, Italy</p> <p>ISBN: 88-87080-59-3</p> <p>pp. 57-85.</p> <p>♣URL: <a href="http://www.edizioniperiferia.it/scheda_libro.php?id_libro=129">http://www.edizioniperiferia.it/scheda_libro.php?id_libro=129</a></p> <p>♣URL: <a href="http://www.silvanapalazzo.it/">http://www.silvanapalazzo.it/</a></p>	<p><b>2006</b></p> 
49.	<p><b>PUTZ M.V.</b></p> <p>Unifying Absolute and Chemical Electronegativity and Hardness Density Functional Formulations through the Chemical Action Concept</p> <p>în</p> <p>"<i>PROGRESS IN QUANTUM CHEMISTRY RESEARCH</i>"</p> <p>Erik O. Hoffman (Ed.)</p> <p>Nova Science Publishers Inc., New York, USA</p> <p>ISBN-10: 1-60021-621-8,</p> <p>ISBN-13: 978-1-60021-621-3,</p> <p>Chapter 2, pp. 59-121.</p> <p>♣URL: <a href="http://www.novapublishers.com/catalog/product_info.php?products_id=5571">http://www.novapublishers.com/catalog/product_info.php?products_id=5571</a></p>	<p><b>2007</b></p> 
50.	<p><b>PUTZ M.V.</b></p> <p>Can Quantum-Mechanical Description of Chemical Bond Be Considered Complete?</p> <p>în "<i>QUANTUM CHEMISTRY RESEARCH TRENDS</i>"</p> <p>Mikas P. Kaisas (Ed.)</p> <p>Nova Science Publishers Inc., New York, USA</p> <p>ISBN-10: 1-60021-620-X; ISBN-13: 978-160021-620-6;</p> <p>Expert Commentary, pp. 3-5.</p> <p>♣URL: <a href="http://www.novapublishers.com/catalog/product_info.php?products_id=5570">http://www.novapublishers.com/catalog/product_info.php?products_id=5570</a></p>	<p><b>2007</b></p> <p><i>"the quantum scenario based on electronegativity and hardness indices and principles stands as a natural first step in developing the quantum chemical space of reactivity"</i></p>

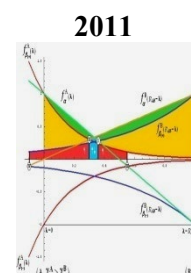
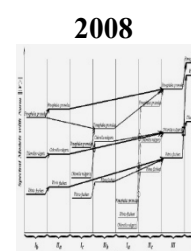


51. **PUTZ M.V., CHIRIAC A.**  
 Quantum Perspectives on the Nature of the Chemical Bond  
 în "*ADVANCES IN QUANTUM CHEMICAL BONDING STRUCTURES*"  
 Mihai V. Putz (Ed.)  
 Transworld Research Network, Kerala, India  
 ISBN: 978-81-7895-306-9; Chapter 1, pp. 1-43  
 ♣URL: <http://www.trnres.com/putz.htm>
52. **PUTZ M.V., DUDA-SEIMAN D., MANCAȘ S., DUDA-SEIMAN C., LACRĂMĂ A.-M.**  
 Quantum and Topological Impact on HMG-CoA Reductase Inhibitors  
 în  
 "*ADVANCES IN QUANTUM CHEMICAL BONDING STRUCTURES*"  
 Mihai V. Putz (Ed.)  
 Transworld Research Network, Kerala, India  
 ISBN: 978-81-7895-306-9; Chapter 15, pp. 355-387  
 ♣URL: <http://www.trnres.com/putz.htm>
53. **LACRĂMĂ A.-M., PUTZ M.V., OSTAFE V.**  
 Designing a Spectral Structure-Activity Ecotoxicologic Battery  
 în  
 "*ADVANCES IN QUANTUM CHEMICAL BONDING STRUCTURES*"  
 Mihai V. Putz (Ed.)  
 Transworld Research Network, Kerala, India  
 ISBN: 978-81-7895-306-9; Chapter 16, pp. 389-419  
 ♣URL: <http://www.trnres.com/putz.htm>
54. **PUTZ M.V.**  
 Fulfilling The Dirac Promises on Quantum Chemical Bond  
 în "*QUANTUM FRONTIERS OF ATOMS AND MOLECULES*"  
 Mihai V. Putz (Ed.)  
 Series,, *Chemistry Research And Applications*”  
 NOVA Science Publishers, Inc., New York, USA  
 ISBN: 978-1-61668-158-6; Chapter 1, pp. 1-20  
 ♣URL: [https://www.novapublishers.com/catalog/product\\_info.php?products\\_id=12687](https://www.novapublishers.com/catalog/product_info.php?products_id=12687)
55. **PUTZ M.V.**  
 Quantum and Electrodynamics Versatility of Electronegativity and Chemical Hardness  
 în  
 "*QUANTUM FRONTIERS OF ATOMS AND MOLECULES*"  
 Mihai V. Putz (Ed.)  
 Series,, *Chemistry Research And Applications*”  
 NOVA Science Publishers, Inc., New York, USA  
 ISBN: 978-1-61668-158-6  
 Chapter 11, pp. 251-270  
 ♣URL: [https://www.novapublishers.com/catalog/product\\_info.php?products\\_id=12687](https://www.novapublishers.com/catalog/product_info.php?products_id=12687)



2008

$$S_{II}^{(n)} = \begin{pmatrix} S_1 & 0 & 1 & \dots & 0 \\ 0 & 1 & S_2 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 1 & 0 & 1 & C_1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \\ \vdots \end{pmatrix}$$



2011

$\eta$	
$\eta^1 = \frac{1}{2} \int_{-1}^1 \frac{1}{\sqrt{1-x^2}} dx$	$\eta^1 = \frac{1}{2} \left( \frac{\partial \eta}{\partial x} \right)_p$
$\eta^2 = \frac{1}{2\sqrt{3}}$	
$\eta^3 = \frac{1}{2} \int_{-1}^1 \frac{1}{\sqrt{1-x^2}} dx$	$\eta^3 = \frac{1}{2} \left( \frac{\partial \eta}{\partial x} \right)_p$
$\eta^4 = \frac{1}{2} \int_{-1}^1 \frac{1}{\sqrt{1-x^2}} dx$	$\eta^4 = \frac{1}{2} \left( \frac{\partial \eta}{\partial x} \right)_p$

56. **PUTZ M.V., PUTZ A.M.**  
 Timisoara Spectral – Structure Activity Relationship (Spectral-SAR) Algorithm:  
 From Statistical and Algebraic Fundamentals to Quantum Consequences  
 în  
 "QUANTUM FRONTIERS OF ATOMS AND MOLECULES"  
 Mihai V. Putz (Ed.)  
 Series,, Chemistry Research And Applications"  
 NOVA Science Publishers, Inc., New York, USA  
 ISBN: 978-1-61668-158-6  
 Chapter 21, pp. 539-580  
 ♣URL:[https://www.novapublishers.com/catalog/product\\_info.php?products\\_id=12687](https://www.novapublishers.com/catalog/product_info.php?products_id=12687)

**2011**

$$\begin{aligned} |Y_{\text{min}}\rangle &= a_1|0\rangle_1 + a_2|1\rangle_1 + \dots + a_n|n-1\rangle_1 + a_n|n\rangle_1 \\ |X_1\rangle &= 1|0\rangle_1 + 0|1\rangle_1 + \dots + 0|n-1\rangle_1 + 0|n\rangle_1 \\ |X_2\rangle &= r_1^2|0\rangle_1 + 1|1\rangle_1 + \dots + 0|n-1\rangle_1 + 0|n\rangle_1 \\ |X_3\rangle &= r_1^4|0\rangle_1 + r_1^2|1\rangle_1 + \dots + 1|n-1\rangle_1 + 0|n\rangle_1 \\ |X_n\rangle &= r_1^{2(n-1)}|0\rangle_1 + r_1^{2(n-2)}|1\rangle_1 + \dots + r_1^2|n-1\rangle_1 + 1|n\rangle_1 \end{aligned}$$

57. **PUTZ M.V.**  
 Conceptual Density Functional Theory: from Inhomogeneous Electronic Gas to  
 Bose-Einstein Condensates  
 în  
 "CHEMICAL INFORMATION AND COMPUTATIONAL CHALLENGES IN 21<sup>ST</sup>  
 CENTURY. A Celebration of 2011 International Year of Chemistry"  
 Mihai V. Putz (Ed.)  
 Series,, Chemistry Research and Applications" &  
 Series ,,Chemical Engineering Methods and Technology"  
 NOVA Science Publishers, Inc., New York, USA  
 ISBN: 978-1-61209-712-1  
 Chapter 1, pp. 1-60  
 ♣URL: [https://www.novapublishers.com/catalog/product\\_info.php?products\\_id=22003](https://www.novapublishers.com/catalog/product_info.php?products_id=22003)

**2011**

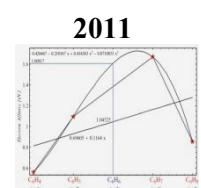
$$\langle (E_{KS}) | \psi(\mathbf{r}) \rangle = - \sum_i E_i \phi_i(\mathbf{r}) \hat{a}_i$$

58. **PUTZ M.V.**  
 Hidden Side of Chemical Bond: The Bosonic Condensate  
 în  
 "ADVANCES IN CHEMISTRY RESEARCH. VOLUME 10"  
 James C. Taylor (Ed.)  
 Series,, Advances in Chemistry Research"  
 NOVA Science Publishers, Inc., New York, USA, ISBN: 978-1-61324-018-2,  
 Chapter 8, pp. 261-298.  
 ♣URL: [https://www.novapublishers.com/catalog/product\\_info.php?products\\_id=22671](https://www.novapublishers.com/catalog/product_info.php?products_id=22671)

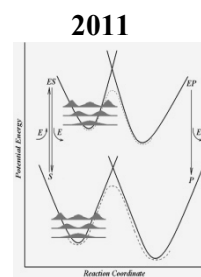
**2011**

$$\underbrace{\Psi_{BB}(\mathbf{r})}_{\text{BOSONIC}} = \underbrace{c_A \Psi_A(\mathbf{r})}_{\text{FERMIONIC SUPERPOSITION}} + \underbrace{c_B \Psi_B(\mathbf{r})}_{\text{FERMIONIC SUPERPOSITION}}$$

59. **PUTZ M.V.**  
 Quantum Parabolic Effects of Electronegativity and Chemical Hardness on  
 Carbon  $\pi$ -Systems  
 în  
 "CARBON BONDING AND STRUCTURES: ADVANCES IN PHYSICS AND  
 CHEMISTRY"  
 Mihai V. Putz (Ed.)  
 Springer Verlag, Dordrecht, NL,  
 ISBN: 978-94-007-1732-9;  
 Series ,,Carbon Materials: Chemistry and Physics",  
 Volume 5  
 Series ISSN: 1875-0745  
 Chapter 1, pp. 1-32; DOI 10.1007/978-94-007-1733-6\_1  
 ♣URL: <http://www.springer.com/chemistry/physical+chemistry/book/978-94-007-1732-9>



60. **PUTZ M.V., PUTZ A.M.**  
 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  
 ISBN 978-1-60960-860-6 (hardcover)  
 ISBN 978-1-60960-861-3 (ebook)  
 ISBN 978-1-60960-862-0 (print & perpetual access)  
 DOI: 10.4018/978-1-60960-860-6.ch007  
 Chapter 7, pp. 168-188  
 ♣URL: <http://www.igi-global.com/bookstore/chapter.aspx?titleid=56454>  
 republicată (de aceeași editură) ca



- PUTZ M.V., PUTZ A.M.**  
 Logistic vs. W-Lambert Information in Quantum Modeling of Enzyme Kinetics  
 în  
 "METHODOLOGIES AND APPLICATIONS FOR CHEMOINFORMATICS AND  
 CHEMICAL ENGINEERING"  
 A. K. Haghi (Ed.)  
 IGI Global(formerly Idea Group Inc.), Hershey, PA 17033, USA  
 ISBN13: 9781466640108; ISBN10: 1466640103; EISBN13: 9781466640115  
 DOI: 10.4018/978-1-4666-4010-8.ch004  
 Chapter 4, pp. 40-59  
 ♣URL: <http://www.igi-global.com/chapter/logistic-lambert-information-quantum-modeling/77068>

2013

61. **PUTZ M.V.**  
 Levels of a Unified Theory of Chemical Interaction  
 în  
 "ADVANCES IN CHEMICAL MODELING",  
 Mihai V. Putz (Ed.)  
 NOVA Science Publishers Inc., New York, USA  
 ISBN: 978-1-61209-028-3; Chapter 1, pp. 1-7  
 ♣URL: [https://www.novapublishers.com/catalog/product\\_info.php?products\\_id=20389](https://www.novapublishers.com/catalog/product_info.php?products_id=20389)

2011

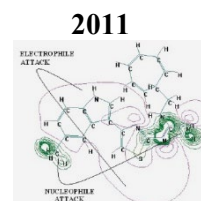
$$\nabla_{\rho}^{\text{eff}}(\rho, \sigma) = \frac{\sum_{L,R} \left[ \sum_{L,R} C_{L,R}^{\text{class}}(\rho, \sigma) + \sum_{L,R} C_{L,R}^{\text{quant}}(\rho, \sigma) \right]}{\sum_{L,R} \left[ \sum_{L,R} C_{L,R}^{\text{class}}(\rho, \sigma) + \sum_{L,R} C_{L,R}^{\text{quant}}(\rho, \sigma) \right]}$$

62. **PUTZ M.V.**  
 Chemical Reactivity and Electromagnetic Field  
 în  
 "ADVANCES IN CHEMICAL MODELING",  
 Mihai V. Putz (Ed.)  
 NOVA Science Publishers Inc., New York, USA  
 ISBN: 978-1-61209-028-3; Chapter 2, pp. 9-14  
 ♣URL: [https://www.novapublishers.com/catalog/product\\_info.php?products\\_id=20389](https://www.novapublishers.com/catalog/product_info.php?products_id=20389)

2011

$$(\text{curl} \otimes \rho) \nabla \times \rightarrow \partial / \partial N; \mathbf{H} \rightarrow E_N$$

63. **PUTZ M.V., DUDA-SEIMAN C., DUDA-SEIMAN D.M., PUTZ A.-M.**  
 Turning SPECTRAL-SAR into 3D-QSAR Analysis. Application on H<sup>+</sup>K<sup>+</sup>-ATPase Inhibitory Activity  
 în  
 "ADVANCES IN CHEMICAL MODELING"  
 Mihai V. Putz (Ed.)  
 NOVA Science Publishers Inc., New York, USA  
 ISBN: 978-1-61209-028-3  
 Chapter 33, pp. 435-451  
 ♣URL: [https://www.novapublishers.com/catalog/product\\_info.php?products\\_id=20389](https://www.novapublishers.com/catalog/product_info.php?products_id=20389)



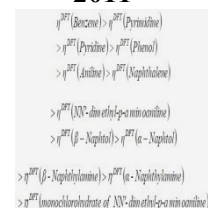
64. **PUTZ M.V.**  
 Chemical Action and the Transition State Reactivity  
 în  
 "ADVANCES IN CHEMICAL MODELING. VOLUME 2"  
 Mihai V. Putz (Ed.)  
 NOVA Science Publishers, Inc., New York, USA  
 ISBN: 978-1-61209-669-8  
 Chapter 2, pp. 27-33  
 ♣URL: [https://www.novapublishers.com/catalog/product\\_info.php?products\\_id=21916](https://www.novapublishers.com/catalog/product_info.php?products_id=21916)

2011

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

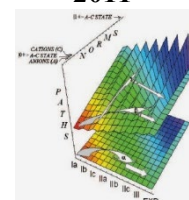
65. **PUTZ M.V., PUTZ A.-M., PITULICE L., CHIRIAC V.**  
 On Chemical Hardness Assessment of Aromaticity for Some Organic Compound  
 în  
 "ADVANCES IN CHEMICAL MODELING. VOLUME 2"  
 Mihai V. Putz (Ed.)  
 NOVA Science Publishers, Inc., New York, USA  
 ISBN: 978-1-61209-669-8  
 Chapter 8, pp. 125-136  
 ♣URL: [https://www.novapublishers.com/catalog/product\\_info.php?products\\_id=21916](https://www.novapublishers.com/catalog/product_info.php?products_id=21916)

2011



66. **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"  
 Mihai V. Putz (Ed.)  
 NOVA Science Publishers, Inc., New York, USA  
 ISBN: 978-1-61209-669-8, Chapter 18, pp. 263-274  
 ♣URL: [https://www.novapublishers.com/catalog/product\\_info.php?products\\_id=21916](https://www.novapublishers.com/catalog/product_info.php?products_id=21916)

2011



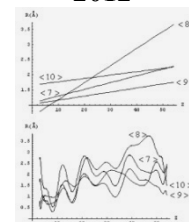
consemnata ca „research summaries” în lucrarea de sinteză

- "CHEMISTRY RESEARCH SUMMARIES. VOLUME 1"  
 Elnur S. Hüseyinov and Vusal Babayev (Eds.)  
 NOVA Science Publishers, Inc., New York, USA  
 ISBN: 978-1-62257-633-3, Chapter 16, pp. 51-52  
 ♣URL: [https://www.novapublishers.com/catalog/product\\_info.php?products\\_id=36712](https://www.novapublishers.com/catalog/product_info.php?products_id=36712)

2012

67. **PUTZ M.V.**  
 Nanoroots of Quantum Chemistry: Atomic Radii, Periodic Behavior, and Bondons  
 în  
 "NANOSCIENCE AND ADVANCING COMPUTATIONAL METHODS IN CHEMISTRY: RESEARCH PROGRESS"  
 E.A. Castro, A. K. Haghi (Editors)  
 IGI Global(formerly Idea Group Inc.), Hershey, PA 17033, USA  
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 ISBN13: 9781466616073, ISBN10: 1466616075, EISBN13: 9781466616080  
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 ♣URL: <http://www.igi-global.com/chapter/nanoroots-quantum-chemistry-atomic-radii/66247>

2012



republicată (de aceeași editură) ca

**PUTZ M.V.**

**2014**

Nanoroots of Quantum Chemistry: Atomic Radii, Periodic Behavior, and Bondons

în "*NANOTECHNOLOGY: CONCEPTS, METHODOLOGIES, TOOLS, AND APPLICATIONS (3 VOLUMES)*"

Information Resources Management Association (USA)

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

DOI: 10.4018/978-1-4666-5125-8.ch005

ISBN13: 9781466651258, ISBN10: 1466651253, EISBN13: 9781466651265

Chapter 5, pp. 123-162

♣URL:<http://www.igi-global.com/book/nanotechnology-concepts-methodologies-tools-applications/90533>

68. **PUTZ M.V., PUTZ A.M.**

**2012**

SPECTRAL-SAR Approach of the Enzymic Activity

în

"*QSAR & SPECTRAL-SAR IN COMPUTATIONAL ECOTOXICOLOGY*",

Mihai V. Putz (Ed.)

Apple Academics, Toronto, Canada

ISBN: 9781926895130

Chapter 2, pp.29-38

URL:<http://www.appleacademicpress.com/title.php?id=50>

Compound Formula	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z
<CH<O>CH<O>	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<CH<O>CH<O>CH<O>	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<CH<O>CH<O>CH<O>CH<O>	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<CH<O>CH<O>CH<O>CH<O>CH<O>	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
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<CH<O>CH<O>CH<O>CH<O>CH<O>CH<O>CH<O>	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
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<CH<O>CH<O>CH<O>CH<O>CH<O>CH<O>CH<O>CH<O>CH<O>CH<O>	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
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69. **PUTZ M.V., PUTZ A.M., OSTAFE V.**

SPECTRAL-SAR Ecotoxicology of Ionic Liquids: The Daphnia Magna Case

în "*QSAR & SPECTRAL-SAR IN COMPUTATIONAL ECOTOXICOLOGY*"

Mihai V. Putz (Ed.)

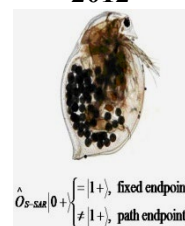
Apple Academics, Toronto, Canada

ISBN: 9781926895130

Chapter 7, pp.133-142

♣URL:<http://www.appleacademicpress.com/title.php?id=50>

**2012**



70. **PUTZ M.V.**

**2012**

Big Chemical Ideas in Context: The Periodic Law and Scerri's Periodic Table

În "*ADVANCES IN CHEMICAL MODELING. VOLUME 3*"

Mihai V. Putz (Ed.)

NOVA Science Publishers, Inc., New York, USA

ISBN: 978-1-62257-110-9, Chapter 1, pp.1-8;

♣URL: [https://www.novapublishers.com/catalog/product\\_info.php?products\\_id=34573](https://www.novapublishers.com/catalog/product_info.php?products_id=34573)

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Period 1	H	He																
Period 2	Li	Be	B	C	N	O	F	Ne										
Period 3	Na	Mg	Al	Si	P	S	Cl	Ar										
Period 4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Period 5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Period 6	Cs	Ba	La	Hf	Ta	W	Re	Os	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
Period 7	Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt									

71. **PUTZ M.V.**

**2012**

On Relationship between Electronic Sharing in Bonding and Electronegativity Equalization of Atoms in Molecules

în

"*ADVANCES IN CHEMICAL MODELING. VOLUME 3*"

Mihai V. Putz (Ed.)

NOVA Science Publishers, Inc., New York, USA

ISBN: 978-1-62257-110-9, Chapter 3, pp.31-46

♣URL: [https://www.novapublishers.com/catalog/product\\_info.php?products\\_id=34573](https://www.novapublishers.com/catalog/product_info.php?products_id=34573)

$$\begin{aligned} & \iint s(r,r') dr dr' \\ &= - \int \left( \frac{\partial}{\partial \chi} \int \rho_{XC}(r,r') dr' \right)_{r(r)} dr \\ &= - \int \left( \frac{\partial \rho(r)}{\partial \chi} \right)_{r(r)} dr \\ &= \int s(r) dr \\ &= S \end{aligned}$$

72. **PUTZ M.V.**, PUTZ A.M., BAROU R.  
Spectral-SAR Realization of OECD-QSAR Principles  
în  
"ADVANCES IN CHEMICAL MODELING. VOLUME 3"  
Mihai V. Putz (Ed.)  
NOVA Science Publishers, Inc., New York, USA  
ISBN: 978-1-62257-110-9, Chapter 32, pp. 449-464  
♣URL: [https://www.novapublishers.com/catalog/product\\_info.php?products\\_id=34573](https://www.novapublishers.com/catalog/product_info.php?products_id=34573)

2012

$$\text{Det}(Y^T X Y) / \text{Det}(X^T X) = 0, \text{Tr} \|A_{\text{REG}}\|$$

$$\hat{\beta}_{\text{LS}} = (X^T X)^{-1} X^T Y = 0, (\alpha, \beta, \gamma, \dots)$$

A.B. PREDICTED ENDPOINTS  
 $\alpha, \beta, \gamma, \dots$  SPECTRAL PATHS

73. **PUTZ M.V.**, IONAȘCU C., CHIRIAC, A.  
Testing Elemental Periodicity by QSPR  
în  
"ADVANCES IN CHEMICAL MODELING. VOLUME 3"  
Mihai V. Putz (Ed.)  
NOVA Science Publishers, Inc., New York, USA  
ISBN: 978-1-62257-110-9  
Chapter 33, pp.465-472  
♣URL: [https://www.novapublishers.com/catalog/product\\_info.php?products\\_id=34573](https://www.novapublishers.com/catalog/product_info.php?products_id=34573)

2012

Model	QSPR	r	r <sup>2</sup> adj
Atom size	2-14(14)4779A	0.9603	0.9407
Radius	2-14(14)3279R	0.8499	0.8207
Molar weight	2-14(14)4009MD	0.8623	0.8377
Density	2-14(14)4027DP	0.8488	0.8247
Depth	2-14(14)1709Y	0.7529	0.6907
EP Electrograph	2-14(14)1679P	0.8079	0.7841
EP Chemical Ionization	2-14(14)2149*2P	0.9468	0.9286
EP Acetate potential	2-14(14)2109*2P	0.8528	0.7987
EP Electro affinity	2-14(14)2099*2P	0.9191	0.9110
DFES Electrograph	2-14(14)1609*2P	0.8937	0.792
DFES Chemical Ionization	2-14(14)2139*2P	0.8959	0.7188
DFES Acetate potential	2-14(14)2119*2P	0.8939	0.7174
DFES Electro affinity	2-14(14)2089*2P	0.8723	0.7119

74. **PUTZ M.V.**  
Chemical Reactivity and Biological Activity Criteria from DFT Parabolic Dependency  $E = E(N)$   
în  
"THEORETICAL AND COMPUTATIONAL DEVELOPMENTS IN MODERN DENSITY FUNCTIONAL THEORY"  
Amlan K. Roy (Ed.)  
NOVA Science Publishers, Inc., New York, USA  
ISBN: 978-1-61942-779-2  
Chapter 17, pp.449-484  
♣URL: [https://www.novapublishers.com/catalog/product\\_info.php?products\\_id=31589](https://www.novapublishers.com/catalog/product_info.php?products_id=31589)

2012

$$F_{\mu} = -\frac{d}{dN}(\mu)$$

$$= -\frac{d}{dN}\left(\frac{E}{N}\right) = \frac{E}{N^2} - \frac{1}{N}\left(\frac{dE}{dN}\right)_{\nu}$$

$$E_{\mu} = \mu N + F_{\mu} N^2$$

$$= -\chi N + \eta N^2$$

75. **PUTZ A.M.**, **PUTZ M.V.**  
Spectral-Structure Activity Relationship (Spectral-SAR) Assessment of Ionic Liquids' in Silico Ecotoxicity  
în  
"IONIC LIQUIDS - NEW ASPECTS FOR THE FUTURE"  
Jun-ichi Kadokawa (Ed.)  
InTech, Inc., Rijeka-New York-Shanghai, Croatia-USA-China  
ISBN: 978-953-51-0937-2  
DOI:10.5772/51657, Chapter 4, pp. 85-126  
♣URL: <http://dx.doi.org/10.5772/51657>

2013



76. **DE CORATO M.**, **BERNASCONI M.**, **D'ALESSIO L.**, **ORI O.**, **PUTZ M.V.**, **BENEDEK G.**  
Topological versus Physical and Chemical Properties of Negatively Curved Carbon Surfaces  
în  
"TOPOLOGICAL MODELING OF NANOSTRUCTURES AND EXTENDED SYSTEMS"  
Ali Reza Ashrafi, Franco Cataldo, Ali Iranmanesh, Ottorino Ori (Eds.)  
Springer Verlag, Dordrecht, NL  
ISBN: 978-94-007-6412-5  
DOI: 10.1007/978-94-007-6413-2\_4, Chapter 4, pp. 105-136  
♣URL: [http://link.springer.com/chapter/10.1007/978-94-007-6413-2\\_7](http://link.springer.com/chapter/10.1007/978-94-007-6413-2_7)

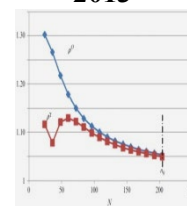
2013

$$\chi^W = \sum_k X_k W^{(k)}$$

$$\eta^W = \sum_k H_k W^{(k)}$$

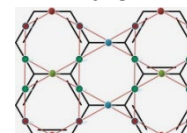
77. **PUTZ M.V.**, DE CORATO M., BENEDEK G., SEDLAR J., GRAOVAC A., ORI O.  
 Topological Invariants of Moebius-Like Graphenic Nanostructures  
 în  
*"TOPOLOGICAL MODELING OF NANOSTRUCTURES AND EXTENDED SYSTEMS"*  
 Ali Reza Ashrafi, Franco Cataldo, Ali Iranmanesh, Ottorino Ori (Eds.)  
 Springer Verlag, Dordrecht, NL  
 ISBN: 978-94-007-6412-5,  
 DOI: 10.1007/978-94-007-6413-2\_7, Chapter 7, pp. 229-244  
 ♣ URL: [http://link.springer.com/chapter/10.1007/978-94-007-6413-2\\_7](http://link.springer.com/chapter/10.1007/978-94-007-6413-2_7)

2013



78. **PUTZ M.V.**, ORI O., DE CORATO M., PUTZ A.M., BENEDEK G., CATALDO F., GRAOVAC A.  
 Introducing „Colored“ Molecular Topology by Reactivity Indices of Electronegativity and Chemical Hardness  
 în  
*"TOPOLOGICAL MODELING OF NANOSTRUCTURES AND EXTENDED SYSTEMS"*  
 Ali Reza Ashrafi, Franco Cataldo, Ali Iranmanesh, Ottorino Ori (Eds.)  
 Springer Verlag, Dordrecht, NL  
 ISBN: 978-94-007-6412-5  
 DOI: 10.1007/978-94-007-6413-2\_9  
 Chapter 9, pp. 265-286  
 ♣ URL: [http://link.springer.com/chapter/10.1007/978-94-007-6413-2\\_9](http://link.springer.com/chapter/10.1007/978-94-007-6413-2_9)

2013



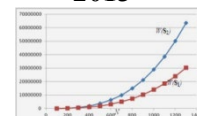
79. **PUTZ M.V.**  
 From Kohn-Sham to Gross-Pitaevsky equation within Bose-Einstein condensation  $\psi$ -theory  
 în  
*"ADVANCES IN CHEMICAL MODELING. VOLUME 4"*  
 Mihai V. Putz (Ed.)  
 NOVA Science Publishers, Inc., New York, USA  
 ISBN: 978-1-62808-186-2  
 Chapter 1, pp. 3-14  
 ♣ URL: [https://www.novapublishers.com/catalog/product\\_info.php?products\\_id=43018](https://www.novapublishers.com/catalog/product_info.php?products_id=43018)

2013

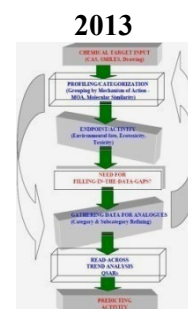
$$\left( -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(\mathbf{r}) + g|\psi(\mathbf{r})|^2 \right) \psi(\mathbf{r}) = \mu \psi(\mathbf{r})$$

80. DE CORATO M., BENEDEK G., ORI O., **PUTZ M.V.**  
 Topological Study of Schwarzitic Junctions in 1D Lattices  
 în  
*"ADVANCES IN CHEMICAL MODELING. VOLUME 4"*  
 Mihai V. Putz (Ed.)  
 NOVA Science Publishers, Inc., New York, USA  
 ISBN: 978-1-62808-186-2  
 Chapter 19; pp. 263-272  
 ♣ URL: [https://www.novapublishers.com/catalog/product\\_info.php?products\\_id=43018](https://www.novapublishers.com/catalog/product_info.php?products_id=43018)

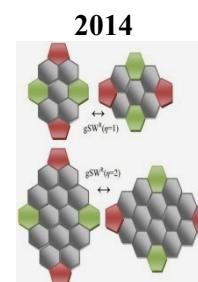
2013



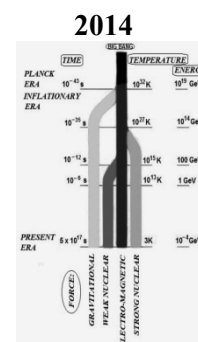
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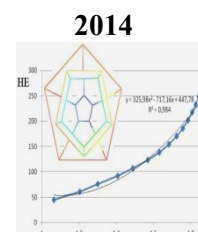
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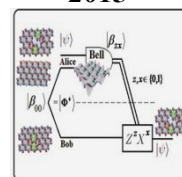
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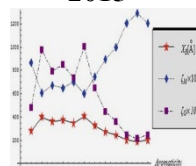


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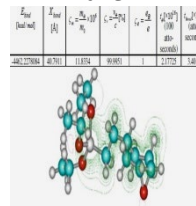
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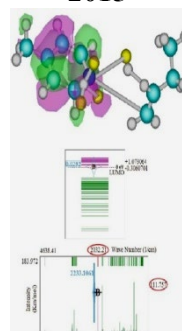
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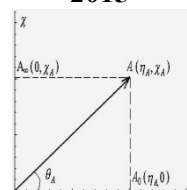


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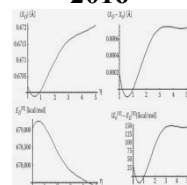
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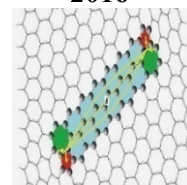
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$$\begin{aligned}
 |F\rangle &= \alpha_0 |X_0\rangle + \alpha_1 |X_1\rangle + \dots + \alpha_M |X_M\rangle \\
 |X_0\rangle &= \hat{S}^{(1)} |X_0\rangle + 0 |X_1\rangle + \dots + 0 |X_M\rangle \\
 |X_1\rangle &= 0 |X_0\rangle + \hat{S}^{(2)} |X_1\rangle + \dots + 0 |X_M\rangle \\
 &\dots \\
 |X_M\rangle &= 0 |X_0\rangle + 0 |X_1\rangle + \dots + \hat{S}^{(M)} |X_M\rangle
 \end{aligned}$$

2016

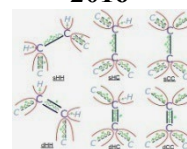


2016

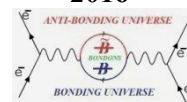


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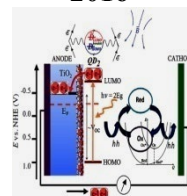
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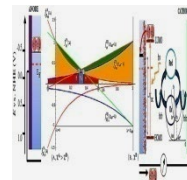
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2016



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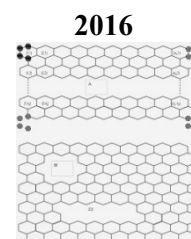
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$$I_n = 2ef = (2e) [18.8177 \times 10^8 \times \Delta \bar{v}_{\text{FERR}} [\text{cm}^{-1}]]$$

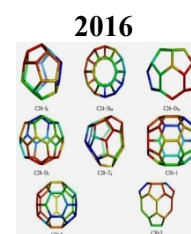
$$V_n = \frac{h}{2e} f = \frac{h}{e} [18.8177 \times 10^8 \times \Delta \bar{v}_{\text{FERR}} [\text{cm}^{-1}]]$$

$$I_{sc} \times V_{oc} = \frac{2\pi h}{IQ} [18.8177 \times 10^8 \times \Delta \bar{v}_{\text{FERR}} [\text{cm}^{-1}]]^2$$

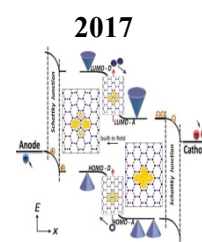
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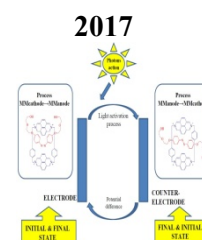
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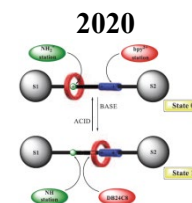
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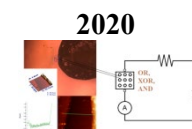
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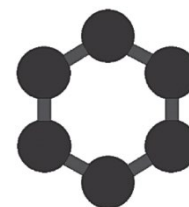
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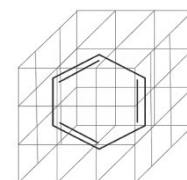
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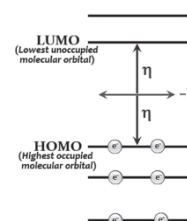
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$$M_B = \frac{\hbar^2}{2E_{bond} X_{bond}^2}$$

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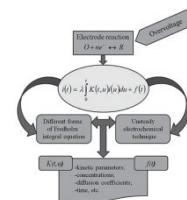
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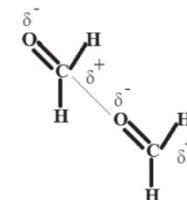
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$$\eta^{MSECHL}(r) = \left\{ \sec h \left[ \sqrt{2} \frac{g(r)}{h(r)} \right] \right\}^{3/2}$$

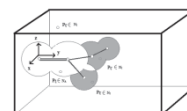
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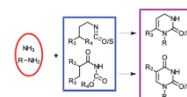
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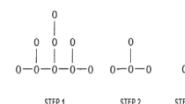
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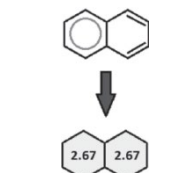
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$$\chi_{\text{Bond-}i\text{-Adjacency}}^{\text{Bond-}i\text{-Adjacency}} = \frac{h_{\text{Bond-}i\text{-Adjacency}}}{\sum_{\text{Type-}i\text{-Bond}} |h_{\text{Type-}i\text{-Bond}}|}$$

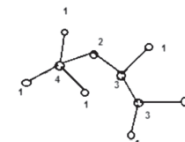
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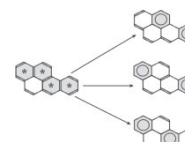
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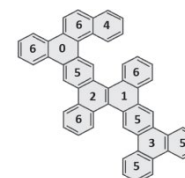
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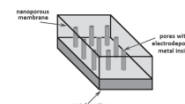
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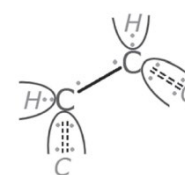
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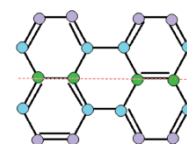
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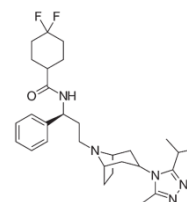
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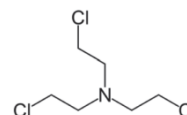
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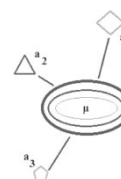
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Software-aided molecular design and QSAR studies have a great potential in designing molecules as therapeutic agents in diabetes mellitus. However, since type 2 diabetes mellitus is a complex disease that includes several biological targets, multi-target QSAR studies are recommended in the future to achieve efficient antidiabetic therapies.

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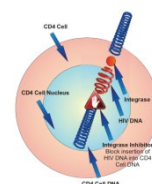
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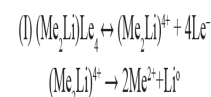
1. HIV gp120 is binding to the CD4 receptor.
2. HIV gp120 suffers a conformational change which increases its affinity for a co-receptor and exposes HIV gp41.
3. HIV gp120 binds to a co-receptor - either CXCR4 or CCR5.
4. HIV gp41 penetrates the HIV lipid membrane and the T cell membrane.
5. The viral core - the capsid is entering into the cell after the fuse of the viral envelope with the cell membrane.

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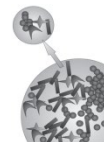
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The Köln model based on the minimum criterion (MCM) is an in vivo biological procedure for toxicological investigation using the minimum plasma of the marine organism *Paracentrotus lividus* (P. lividus) from the Sicily specific to the station until the voluntary uptake (stable phase). The effluents experiments with crude oils, components, and surfactants show that the organism is suitable also for toxicity determinations from this domain especially in case of accidents by offshore or territorial drilling, transport by piping procedures termed "operational discharge," or by petroleum industrial accident. The MCM is simple, fast, reproducible, and meets the "3R" requirements regarding the usage of the animal in laboratory experiments.

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$$A_i = \alpha - \beta MSD_i$$

$$MSD_i = \sum_{j=1}^m d_j |w_{ij} x_{ij} - v_j|$$

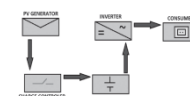
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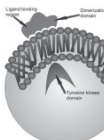
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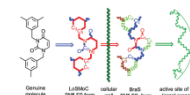
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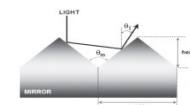
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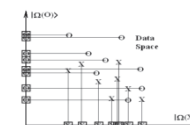
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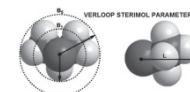
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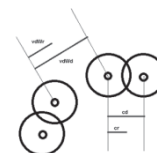
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$$\log \left( \frac{k_s}{k_{CH_3}} \right) = \delta E_s$$

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