Mihai V Putz

List of Publications by Year
in descending order

137 papers	1,768 citations	236612 25 h-index	360668 35 g-index
142 all docs	142 docs citations	142 times ranked	1201 citing authors

#	Article	IF	Citations
1	About the Mulliken electronegativity in DFT. Theoretical Chemistry Accounts, 2005, 114, 38-45.	0.5	104
2	Atomic Radii Scale and Related Size Properties from Density Functional Electronegativity Formulation. Journal of Physical Chemistry A, 2003, 107, 5461-5465.	1.1	65
3	Spectral Inverse Quantum (Spectral-IQ) Method for Modeling Mesoporous Systems: Application on Silica Films by FTIR. International Journal of Molecular Sciences, 2012, 13, 15925-15941.	1.8	57
4	On the applicability of the HSAB principle through the use of improved computational schemes for chemical hardness evaluation. Journal of Computational Chemistry, 2004, 25, 994-1003.	1.5	56
5	The Bondons: The Quantum Particles of the Chemical Bond. International Journal of Molecular Sciences, 2010, 11, 4227-4256.	1.8	56
6	Systematic formulations for electronegativity and hardness and their atomic scales within density functional softness theory. International Journal of Quantum Chemistry, 2006, 106, 361-389.	1.0	54
7	A Spectral-SAR Model for the Anionic-Cationic Interaction in Ionic Liquids: Application to Vibrio fischeri Ecotoxicity. International Journal of Molecular Sciences, 2007, 8, 842-863.	1.8	50
8	Density Functionals of Chemical Bonding. International Journal of Molecular Sciences, 2008, 9, 1050-1095.	1.8	49
9	Linear and Branched PEIs (Polyethylenimines) and Their Property Space. International Journal of Molecular Sciences, 2016, 17, 555.	1.8	49
10	Introducing Spectral Structure Activity Relationship (S-SAR) Analysis. Application to Ecotoxicology. International Journal of Molecular Sciences, 2007, 8, 363-391.	1.8	44
11	Topological Anisotropy of Stone-Wales Waves in Graphenic Fragments. International Journal of Molecular Sciences, 2011, 12, 7934-7949.	1.8	38
12	Bondonic characterization of extended nanosystems: Application to grapheneâ€™s nanoribbons. Chemical Physics Letters, 2012, 548, 95-100.	1.2	37
13	Electronegativity and Chemical Hardness: Different Patterns in Quantum Chemistry. Current Physical Chemistry, 2011, 1, 111-139.	0.1	36
14	Markovian approach of the electron localization functions. International Journal of Quantum Chemistry, 2005, 105, 1-11.	1.0	35
15	Electronegativity: Quantum observable. International Journal of Quantum Chemistry, 2009, 109, 733-738.	1.0	35
16	Chemical action and chemical bonding. Computational and Theoretical Chemistry, 2009, 900, 64-70.	1.5	32
17	Alert-QSAR. Implications for Electrophilic Theory of Chemical Carcinogenesis. International Journal of Molecular Sciences, 2011, 12, 5098-5134.	1.8	32
18	Path Integrals for Electronic Densities, Reactivity Indices, and Localization Functions in Quantum Systems. International Journal of Molecular Sciences, 2009, 10, 4816-4940.	1.8	31

#	ARTICLE	IF	CITATIONS
19	Determining Chemical Reactivity Driving Biological Activity from SMILES Transformations: The Bonding Mechanism of Anti-HIV Pyrimidines. Molecules, 2013, 18, 9061-9116.	1.7	31
20	Bondonic Effects in Group-IV Honeycomb Nanoribbons with Stone-Wales Topological Defects. Molecules, 2014, 19, 4157-4188.	1.7	31
21	New Link between Conceptual Density Functional Theory and Electron Delocalization. Journal of Physical Chemistry A, 2011, 115, 12459-12462.	1.1	30
22	Effect of the Polysaccharide Extract from the Edible Mushroom Pleurotus ostreatus against Infectious Bursal Disease Virus. International Journal of Molecular Sciences, 2009, 10, 3616-3634.	1.8	29
23	Quantum-SAR Extension of the Spectral-SAR Algorithm. Application to Polyphenolic Anticancer Bioactivity. International Journal of Molecular Sciences, 2009, 10, 1193-1214.	1.8	29
24	Chemical Structure-Biological Activity Models for Pharmacophoresâ€™ 3D-Interactions. International Journal of Molecular Sciences, 2016, 17, 1087.	1.8	29
25	SEMICLASSICAL ELECTRONEGATIVITY AND CHEMICAL HARDNESS. Journal of Theoretical and Computational Chemistry, 2007, 06, 33-47.	1.8	28
26	KÃ¶ln-TimiÅŸoara Molecular Activity Combined Models toward Interspecies Toxicity Assessment. International Journal of Molecular Sciences, 2009, 10, 4474-4497.	1.8	27
27	Full Analytic Progress Curves of Enzymic Reactions in Vitro. International Journal of Molecular Sciences, 2006, 7, 469-484.	1.8	26
28	Variational principles for mechanistic quantitative structureâ€“activity relationship (QSAR) studies: application on uracil derivativesâ€™ anti-HIV action. Structural Chemistry, 2013, 24, 1873-1893.	1.0	26
29	Parabolic Reactivity â€œColoringâ€•Molecular Topology: Application to Carcinogenic PAHs. Current Organic Chemistry, 2013, 17, 2816-2830.	0.9	24
30	Compactness Aromaticity of Atoms in Molecules. International Journal of Molecular Sciences, 2010, 11, 1269-1310.	1.8	23
31	Learning the Relationship between the Primary Structure of HIV Envelope Glycoproteins and Neutralization Activity of Particular Antibodies by Using Artificial Neural Networks. International Journal of Molecular Sciences, 2016, 17, 1710.	1.8	21
32	Koopmans' Analysis of Chemical Hardness with Spectral-Like Resolution. Scientific World Journal, The, 2013, 2013, 1-14.	0.8	19
33	Variational perturbation theory for Markov processes. Physical Review E, 2002, 65, 066128.	0.8	18
34	On electronegativity and chemical hardness relationships with aromaticity. Journal of Mathematical Chemistry, 2010, 47, 487-495.	0.7	17
35	Residual-QSAR. Implications for genotoxic carcinogenesis. Chemistry Central Journal, 2011, 5, 29.	2.6	17
36	Predicting bondons by <scp>G</scp>oldstone mechanism with chemical topological indices. International Journal of Quantum Chemistry, 2015, 115, 137-143.	1.0	17

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37	Electrophilicity kernel and its hierarchy through softness in conceptual density functional theory. International Journal of Quantum Chemistry, 2013, 113, 2163-2171.	1.0	16
38	Isomeric Formation of 5|8|5 Defects in Graphenic Systems. Fullerenes Nanotubes and Carbon Nanostructures, 2014, 22, 887-900.	1.0	16
39	Design of Anti-HIV Ligands by Means of Minimal Topological Difference (MTD) Method. International Journal of Molecular Sciences, 2006, 7, 537-555.	1.8	15
40	Density Functional Theory of Boseâ€“Einstein Condensation: Road to Chemical Bonding Quantum Condensate. Structure and Bonding, 2012, , 1-49.	1.0	15
41	Topological Organic Chemistry: From Distance Matrix to Timisoara Eccentricity. Current Organic Chemistry, 2015, 19, 249-273.	0.9	15
42	A new route to graphene starting from heavily ozonized fullerenes: Part 1â€”thermal reduction under inert atmosphere. Fullerenes Nanotubes and Carbon Nanostructures, 2016, 24, 52-61.	1.0	14
43	DFT Chemical Reactivity Driven by Biological Activity: Applications for the Toxicological Fate of Chlorinated PAHs. Structure and Bonding, 2013, , 181-231.	1.0	13
44	Cooperative topological accumulation of vacancies in honeycomb lattices. Fullerenes Nanotubes and Carbon Nanostructures, 2016, 24, 353-362.	1.0	13
45	On Heisenberg Uncertainty Relationship, Its Extension, and the Quantum Issue of Wave-Particle Duality. International Journal of Molecular Sciences, 2010, 11, 4124-4139.	1.8	12
46	A new route to graphene starting from heavily ozonized fullerenes: Part 3 â€“ an electron spin resonance study. Fullerenes Nanotubes and Carbon Nanostructures, 2016, 24, 195-201.	1.0	12
47	Quantitative structureâ€“activity/ecotoxicity relationships (QSAR/QEcoSAR) of a series of phosphonates. Environmental Toxicology and Pharmacology, 2015, 40, 800-824.	2.0	11
48	Noble gas endohedral fullerenes, Ng@C60 (Ng=Ar, Kr): a particular benchmark for assessing the account of non-covalent interactions by density functional theory calculations. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	11
49	A new route to graphene starting from heavily ozonized fullerenes: Part 2â€”oxidation in air. Fullerenes Nanotubes and Carbon Nanostructures, 2016, 24, 62-66.	1.0	11
50	Molecular Graph Theory: From Adjacency Information to Colored Topology by Chemical Reactivity. Current Organic Chemistry, 2015, 19, 359-386.	0.9	11
51	On the Reducible Character of Haldane-RadiÄ‡ Enzyme Kinetics to Conventional and Logistic Michaelis-Menten Models. Molecules, 2011, 16, 3128-3145.	1.7	10
52	Structure Properties and Chemical-Bio/Ecological of PAH Interactions: From Synthesis to Cosmic Spectral Lines, Nanochemistry, and Lipophilicity-Driven Reactivity. Current Organic Chemistry, 2013, 17, 2845-2871.	0.9	10
53	Topological Invariants of Nanocones and Fullerenes. Current Organic Chemistry, 2015, 19, 240-248.	0.9	10
54	Introducing Catastrophe-QSAR. Application on Modeling Molecular Mechanisms of Pyridinone Derivative-Type HIV Non-Nucleoside Reverse Transcriptase Inhibitors. International Journal of Molecular Sciences, 2011, 12, 9533-9569.	1.8	9

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55	Molecular Dynamic Studies of the Complex Polyethylenimine and Glucose Oxidase. International Journal of Molecular Sciences, 2016, 17, 1796.	1.8	9
56	Topological Symmetry Transition between Toroidal and Klein Bottle Graphenic Systems. Symmetry, 2020, 12, 1233.	1.1	9
57	Quantum Parabolic Effects of Electronegativity and Chemical Hardness on Carbon Ï€-Systems. Carbon Materials, 2011, , 1-32.	0.2	9
58	Bondonic Chemistry: Physical Origins and Entanglement Prospects. Carbon Materials, 2015, , 229-260.	0.2	9
59	Quantitative Structure Inter-Activity Relationship (QSInAR). Cytotoxicity Study of Some Hemisynthetic and Isolated Natural Steroids and Precursors on Human Fibrosarcoma Cells HT1080. Molecules, 2011, 16, 6603-6620.	1.7	8
60	Ligand Shaping in Induced Fit Docking of MraY Inhibitors. Polynomial Discriminant and Laplacian Operator as Biological Activity Descriptors. International Journal of Molecular Sciences, 2017, 18, 1377.	1.8	8
61	Generalized topological efficiency â€“ case study with C₈₄ fullerene. Fullerenes Nanotubes and Carbon Nanostructures, 2020, 28, 545-550.	1.0	8
62	Valence atom with bohmian quantum potential: the golden ratio approach. Chemistry Central Journal, 2012, 6, 135.	2.6	7
63	Double Variational Bindingâ€"(SMILES) Conformational Analysis by Docking Mechanisms for Anti-HIV Pyrimidine Ligands. International Journal of Molecular Sciences, 2015, 16, 19553-19601.	1.8	7
64	Surface modification of activated carbon fabric with ozone. Part 2: Thermal analysis with TGA-FTIR and DTA. Fullerenes Nanotubes and Carbon Nanostructures, 2016, 24, 400-405.	1.0	7
65	Quantum particles on graphenic systems. Part 2. Bondons by absorption Raman spectra. Fullerenes Nanotubes and Carbon Nanostructures, 2018, 26, 330-341.	1.0	7
66	Fock-Space Coupled Cluster Theory: Systematic Study of Partial Fourth Order Triples Schemes for Ionization Potential and Comparison with Bondonic Formalism. International Journal of Molecular Sciences, 2020, 21, 6199.	1.8	7
67	Mitotic Checkpoint Proteins Mad1 and Mad2 â€“ Structural and Functional Relationship with Implication in Genetic Diseases. Current Computer-Aided Drug Design, 2014, 10, 168-181.	0.8	6
68	Bondonic Chemistry: Spontaneous Symmetry Breaking of the Topo-reactivity on Graphene. Carbon Materials, 2016, , 345-389.	0.2	6
69	Surface modification of activated carbon fabric with ozone, part 1: Kinetics and oxidation degree. Fullerenes Nanotubes and Carbon Nanostructures, 2016, 24, 313-323.	1.0	6
70	Face colorings and chiral face colorings of icosahedral giant fullerenes: C80 to C240. Fullerenes Nanotubes and Carbon Nanostructures, 2021, 29, 1-12.	1.0	6
71	Chemical Bonding by the Chemical Orthogonal Space of Reactivity. International Journal of Molecular Sciences, 2021, 22, 223.	1.8	6
72	Spectral SAR Ecotoxicology of Ionic Liquids: TheDaphnia magnaCase. Research Letters in Ecology, 2007, 2007, 1-5.	0.6	5

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73	SPECTRAL VS. STATISTIC APPROACH OF STRUCTUREâ€“ACTIVITY RELATIONSHIP. APPLICATION ON ECOTOXICITY OF ALIPHATIC AMINES. Journal of Theoretical and Computational Chemistry, 2009, 08, 1235-1251.	1.8	5
74	Bondonic Chemistry: Predicting Ionic Liquidsâ€™ (IL) Bondons by Raman-IR Spectra. Carbon Materials, 2015, , 347-381.	0.2	5
75	On The Action of Ozone on Single-Wall Carbon Nanohorns (SWCNH). Fullerenes Nanotubes and Carbon Nanostructures, 2015, 23, 1095-1102.	1.0	5
76	Geometry and Topology of Nanotubes and Nanotori. Carbon Materials, 2015, , 131-152.	0.2	5
77	Bondonic Chemistry: Consecrating Silanes as Metallic Precursors for Silicenes Materials. Carbon Materials, 2015, , 323-345.	0.2	5
78	MTD-comsia modelling of HMG-CoA reductase inhibitors. Journal of the Serbian Chemical Society, 2011, 76, 85-99.	0.4	4
79	ON QUANTITATIVE STRUCTUREâ€“TOXICITY RELATIONSHIPS (QSTR) USING HIGH CHEMICAL DIVERSITY MOLECULES GROUP. Journal of Theoretical and Computational Chemistry, 2012, 11, 265-272.	1.8	4
80	Topological Efficiency of Fullerene. Journal of Computational and Theoretical Nanoscience, 2015, 12, 971-975.	0.4	4
81	Surface modification of activated carbon fabric with ozone. Part 3: Thermochemical aspects and electron spin resonance. Fullerenes Nanotubes and Carbon Nanostructures, 2016, 24, 406-413.	1.0	4
82	From graphyne to cata-condensed (Acenographynes) and peri-condensed PAHs-graphyne derivatives. Fullerenes Nanotubes and Carbon Nanostructures, 2018, 26, 535-544.	1.0	4
83	Atoms in Generalized Orbital Configurations: Towards Atom-Dedicated Density Functionals. International Journal of Molecular Sciences, 2019, 20, 5943.	1.8	4
84	Molecular Devices and Machines: Hybrid Organic-Inorganic Structures. Current Organic Chemistry, 2018, 21, .	0.9	4
85	Protein Interaction with Dendrimer Monolayers: Energy and Surface Topology. Symmetry, 2020, 12, 641.	1.1	3
86	Combinatorics of chiral and stereo isomers of substituted nanotubes: applications of Eulerian character indices and comparison with bondonic formalism. Fullerenes Nanotubes and Carbon Nanostructures, 0, , 1-19.	1.0	3
87	Three-Body Excitations in Fock-Space Coupled-Cluster: Fourth Order Perturbation Correction to Electron Affinity and Its Relation to Bondonic Formalism. International Journal of Molecular Sciences, 2021, 22, 8953.	1.8	3
88	Neurotoxicity of Pesticides: The Roadmap for the Cubic Mode of Action. Current Medicinal Chemistry, 2020, 27, 54-77.	1.2	3
89	Topological Modeling of Carbon Nano-lattices. Current Organic Chemistry, 2018, 21, .	0.9	3
90	Chemical Field Theory: The Inverse Density Problem of Electronegativity and Chemical Hardness for Chemical Bond. Current Physical Chemistry, 2017, 7, .	0.1	3

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91	Quantum Dots Searching for Bondots. Advances in Chemical and Materials Engineering Book Series, 2017, , 261-327.	0.2	3
92	Structureâ€“Biological Function Relationship Extended to Mitotic Arrest-Deficient 2-Like Protein Mad2 Native and Mutants-New Opportunity for Genetic Disorder Control. International Journal of Molecular Sciences, 2014, 15, 21381-21400.	1.8	2
93	Computational Modeling of Physical and Chemical Properties of Nanomaterials. Journal of Nanomaterials, 2015, 2015, 1-2.	1.5	2
94	An Algebraic Modification of Wiener and Hyperâ€“Wiener Indices and Their Calculations for Fullerenes. Carbon Materials, 2016, , 33-50.	0.2	2
95	Quantum particles on graphenic systems. Part 1. roadmap for semiconductor based graphenes. Fullerenes Nanotubes and Carbon Nanostructures, 2018, 26, 303-314.	1.0	2
96	Bondonic Chemistry: Non-classical Implications on Classical Carbon Systems. Carbon Materials, 2015, , 261-322.	0.2	2
97	Sustainable Design of Photovoltaics. Advances in Chemical and Materials Engineering Book Series, 2017, , 412-489.	0.2	2
98	Quantum Metrological Matrices for Sustainable Graphentronics. Springer Proceedings in Energy, 2020, , 315-326.	0.2	2
99	Chemical bonding as quantum tunneling: The Capra bondons. Fullerenes Nanotubes and Carbon Nanostructures, 2022, 30, 979-986.	1.0	2
100	Logistic vs. W-Lambert Information in Quantum Modeling of Enzyme Kinetics. International Journal of Chemoinformatics and Chemical Engineering, 2011, 1, 42-60.	0.1	1
101	Hydractinia echinata test-system. IV. Toxic synergism of human pharmaceuticals in mixtures with iodoform. Ecotoxicology and Environmental Safety, 2016, 134, 80-85.	2.9	1
102	Carbon-based specific adjacency-in-bonding (SAIB) isomerism driving aromaticity. Fullerenes Nanotubes and Carbon Nanostructures, 2016, 24, 733-748.	1.0	1
103	Chemical reactivity driving switchable molecular machines. A case of Bipyridine -Calixarene rotaxane. Fullerenes Nanotubes and Carbon Nanostructures, 2019, 27, 514-524.	1.0	1
104	Clef topo-toxicity by cubic representations of organophosphates. Fullerenes Nanotubes and Carbon Nanostructures, 2019, 27, 167-188.	1.0	1
105	Introducing â€œColoredâ€•Molecular Topology by Reactivity Indices of Electronegativity and Chemical Hardness. Carbon Materials, 2013, , 265-286.	0.2	1
106	QSAR by Minimal Topological Difference[s]: Post-Modern Perspectives. Current Medicinal Chemistry, 2020, 27, 42-53.	1.2	1
107	Editorial (Thematic Issue: Polycyclic Aromatic Hydrocarbons: From Structure to Chemical Reactivity) Tj ETQq1 1 0.784314 rgBT /Overl	0.9	1
108	QSTR Studies Regarding the ECOSAR Toxicity of Benzene-Carboxylic Acid' Esters to Fathead Minnow Fish (Pimephales promelas). Current Computer-Aided Drug Design, 2014, 10, 99-106.	0.8	1

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109	Bondonic Electrochemistry. Advances in Chemical and Materials Engineering Book Series, 2017, , 328-411.	0.2	1
110	Quantum Dots Searching for Bondots. , 2017, , 1805-1874.		1
111	Electronic Structure of Linear Polyacenes. Current Organic Chemistry, 2018, 21, .	0.9	1
112	The Density Functional Theory Account of Interplaying Long-Range Exchange and Dispersion Effects in Supramolecular Assemblies of Aromatic Hydrocarbons with Spin. Molecules, 2022, 27, 45.	1.7	1
113	Editorial (Thematic Issue: Current Challenges in QSAR/QSPR Analysis). Current Computer-Aided Drug Design, 2014, 10, 97-98.	0.8	0
114	Developing density functional theory for Bose-Einstein condensates. The case of chemical bonding. , 2015, , .		0
115	Editorial (Thematic Issue: Graph Theory and Molecular Topology in Organic Chemistry ~ Part 2) Tj ETQq1 1 0.784314 rgBT /Ove	0.9	0
116	New Keys for Old Keywords: Hybridization and Aromaticity, Graphs and Topology. , 2018, , 389-501.		0
117	Bond! Chemical Bond: Electronic Structure Methods at Work. , 2018, , 291-388.		0
118	Atomic Structure and Quantum Mechanics. , 2018, , 1-106.		0
119	Density Functional Theory: From Conceptual Level Toward Practical Functionality. , 2018, , 221-289.		0
120	Bonding in Rings and Clusters. , 2018, , 681-723.		0
121	Add on. The Bondon: A New Theory of Electron Effective Coupling and Density Ensembles. , 2018, , 725-782.		0
122	Editorial: Sustainable Organic and Hybrid Nanomaterials: From Structure to Functions. Current Organic Chemistry, 2018, 21, .	0.9	0
123	Molecular Modeling: From Chemical-biological Structure to Pharmaco- medical Activity and Function. Current Medicinal Chemistry, 2020, 27, 3-4.	1.2	0
124	Challenging the HSAB principle on molecular machinesâ€™ precursors. Fullerenes Nanotubes and Carbon Nanostructures, 0, , 1-13.	1.0	0
125	Carbon nano-clustering introducing quantum management. Fullerenes Nanotubes and Carbon Nanostructures, 0, , 1-9.	1.0	0
126	Editorial (Thematic Issue: Graph Theory and Molecular Topology in Organic Chemistry ~ Part 1 ~). Current Organic Chemistry, 2015, 19, 204-204.	0.9	0

#	Article	IF	Citations
127	Bondonic Electrochemistry. , 2017, , 277-359.		0
128	Sustainable Design of Photovoltaics. , 2017, , 416-493.		0
129	Atlas of ï¸ ïŁ, and TMâ€“EC for Fullerenes Isomers. Advances in Chemical and Materials Engineering Book Series, 2017, , 615-656.	0.2	0
130	Entropy of Nanostructures. Advances in Chemical and Materials Engineering Book Series, 2017, , 600-614.	0.2	0
131	Ld/Mm+ Simulation of Some Aristolochic and Humic Acids Species Coupled in Periodic Box with Water. Current Computer-Aided Drug Design, 2021, 17, 708-724.	0.8	0
132	Nanoroots of Quantum Chemistry Atomic Radii, Periodic Behavior, and Bondons. , 0, , 103-143.		0
133	Logistic vs. W-Lambert Information in Quantum Modeling of Enzyme Kinetics. , 0, , 40-59.		0
134	Nanoroots of Quantum Chemistry. , 0, , 123-162.		0
135	Logistic vs. W-Lambert Information in Modeling Enzyme Kinetics at Quantum Level. , 0, , 1413-1431.		0
136	Logistic vs. W-Lambert Information in Modeling Enzyme Kinetics at Quantum Level. , 0, , 168-188.		0
137	Quantum fluctuations on matriceal graphenic heterojunctions e-circuits. Fullerenes Nanotubes and Carbon Nanostructures, 0, , 1-9.	1.0	0