Patrick Bultinck

List of Publications by Year
in descending order

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208 papers	7,968 citations	50276 46 h-index	69250 77 g-index
212 all docs	212 docs citations	212 times ranked	5511 citing authors

#	Article	IF	Citations
1	Critical analysis and extension of the Hirshfeld atoms in molecules. Journal of Chemical Physics, 2007, 126, 144111.	3.0	577
2	Multicenter bond indices as a new measure of aromaticity in polycyclic aromatic hydrocarbons. Journal of Physical Organic Chemistry, 2005, 18, 706-718.	1.9	365
3	A Confidence Level Algorithm for the Determination of Absolute Configuration Using Vibrational Circular Dichroism or Raman Optical Activity. ChemPhysChem, 2011, 12, 1542-1549.	2.1	184
4	Electron Delocalization and Aromaticity in Linear Polyacenes:â€‰ Atoms in Molecules Multicenter Delocalization Index. Journal of Physical Chemistry A, 2006, 110, 7642-7648.	2.5	176
5	A New Mean-Field Method Suitable for Strongly Correlated Electrons: Computationally Facile Antisymmetric Products of Nonorthogonal Geminals. Journal of Chemical Theory and Computation, 2013, 9, 1394-1401.	5.3	166
6	Critical thoughts on computing atom condensed Fukui functions. Journal of Chemical Physics, 2007, 127, 034102.	3.0	162
7	Critical analysis of the local aromaticity concept in polyaromatic hydrocarbons. Faraday Discussions, 2007, 135, 347-365.	3.2	156
8	Uniqueness and basis set dependence of iterative Hirshfeld charges. Chemical Physics Letters, 2007, 444, 205-208.	2.6	136
9	The Electronegativity Equalization Method I: Parametrization and Validation for Atomic Charge Calculations. Journal of Physical Chemistry A, 2002, 106, 7887-7894.	2.5	123
10	Electron delocalization and aromaticity in low-lying excited states of archetypal organic compounds. Physical Chemistry Chemical Physics, 2011, 13, 20690.	2.8	116
11	Analyzing Toxicity Through Electrophilicity. Molecular Diversity, 2006, 10, 119-131.	3.9	115
12	Negative Fukui functions: New insights based on electronegativity equalization. Journal of Chemical Physics, 2003, 118, 4349-4356.	3.0	114
13	Electrostatic Potentials from Self-Consistent Hirshfeld Atomic Charges. Journal of Chemical Theory and Computation, 2009, 5, 334-340.	5.3	112
14	Molecular Quantum Similarity: Theory and Applications. Reviews in Computational Chemistry, 2005, , 127-207.	1.5	105
15	Correlation of Delocalization Indices and Currentâ€Ðensity Maps in Polycyclic Aromatic Hydrocarbons. Chemistry - A European Journal, 2008, 14, 3093-3099.	3.3	100
16	The Electronegativity Equalization Method II: Applicability of Different Atomic Charge Schemes. Journal of Physical Chemistry A, 2002, 106, 7895-7901.	2.5	99
17	Six questions on topology in theoretical chemistry. Computational and Theoretical Chemistry, 2015, 1053, 2-16.	2.5	99
18	Information-Theoretic Approaches to Atoms-in-Molecules: Hirshfeld Family of Partitioning Schemes. Journal of Physical Chemistry A, 2018, 122, 4219-4245.	2.5	97

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19	Efficient description of strongly correlated electrons with mean-field cost. Physical Review B, 2014, 89, .	3.2	95
20	Aliovalent doping of CeO₂: DFT study of oxidation state and vacancy effects. Journal of Materials Chemistry A, 2014, 2, 13723-13737.	10.3	93
21	Local Aromaticity in Polycyclic Aromatic Hydrocarbons: Electron Delocalization versus Magnetic Indices. Chemistry - A European Journal, 2006, 12, 8813-8818.	3.3	90
22	The influence of orbital rotation on the energy of closed-shell wavefunctions. Molecular Physics, 2014, 112, 853-862.	1.7	84
23	A size-consistent approach to strongly correlated systems using a generalized antisymmetrized product of nonorthogonal geminals. Computational and Theoretical Chemistry, 2013, 1003, 101-113.	2.5	81
24	Multidimensionality of delocalization indices and nucleus independent chemical shifts in polycyclic aromatic hydrocarbons. Journal of Computational Chemistry, 2008, 29, 358-366.	3.3	80
25	Quantum Mechanical Basis for Mulliken Population Analysis. Journal of Mathematical Chemistry, 2004, 36, 231-239.	1.5	74
26	Extending Hirshfeldâ€‰to bulk and periodic materials. Journal of Computational Chemistry, 2013, 34, 405-417.	3.3	72
27	Solvent effects on IR and VCD spectra of natural products: an experimental and theoretical VCD study of pulegone. Physical Chemistry Chemical Physics, 2008, 10, 3498.	2.8	68
28	Projected seniority-two orbital optimization of the antisymmetric product of one-reference orbital geminal. Journal of Chemical Physics, 2014, 140, 214114.	3.0	68
29	A VCD robust mode analysis of induced chirality: The case of pulegone in chloroform. Chirality, 2009, 21, E287-97.	2.6	63
30	A Mathematical Discussion on Density and Shape Functions, Vector Semispaces and Related Questions. Journal of Mathematical Chemistry, 2004, 36, 191-200.	1.5	61
31	Can the current density map topology be extracted from the nucleus independent chemical shifts?. Physical Chemistry Chemical Physics, 2016, 18, 11746-11755.	2.8	61
32	Determination of the Stereochemistry of 3-Hydroxymethyl-2,3-dihydro-[1,4]dioxino[2,3-b]- pyridine by Vibrational Circular Dichroism and the Effect of DFT Integration Grids. Journal of Physical Chemistry A, 2003, 107, 542-553.	2.5	60
33	Induced solvent chirality: A VCD study of camphor in CDCl3. Chemical Physics Letters, 2008, 450, 426-430.	2.6	60
34	Variational determination of the second-order density matrix for the isoelectronic series of beryllium, neon, and silicon. Physical Review A, 2009, 80, .	2.5	59
35	Nonvariational Orbital Optimization Techniques for the AP1roG Wave Function. Journal of Chemical Theory and Computation, 2014, 10, 4873-4882.	5.3	59
36	Aromaticity in heterocyclic analogues of benzene: comprehensive analysis of structural aspects, electron delocalization and magnetic characteristics. Physical Chemistry Chemical Physics, 2011, 13, 20536.	2.8	58

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37	Negative and Infinite Fukui Functions: The Role of Diagonal Dominance in the Hardness Matrix. Journal of Mathematical Chemistry, 2003, 34, 67-74.	1.5	56
38	Comparison of the Hirshfeld-I and iterated stockholder atoms in molecules schemes. Physical Chemistry Chemical Physics, 2009, 11, 3424.	2.8	54
39	Stereochemistry of the Tadalafil Diastereoisomers: A Critical Assessment of Vibrational Circular Dichroism, Electronic Circular Dichroism, and Optical Rotatory Dispersion. Journal of Medicinal Chemistry, 2013, 56, 8903-8914.	6.4	54
40	The Fukui matrix: a simple approach to the analysis of the Fukui function and its positive character. Physical Chemistry Chemical Physics, 2011, 13, 6110.	2.8	53
41	Removal of the Pyridine Directing Group from Î±-Substituted N-(Pyridin-2-yl)piperidines Obtained via Directed Ru-Catalyzed sp³ Câ€“H Functionalization. Journal of Organic Chemistry, 2013, 78, 9803-9814.	3.2	53
42	How to Compute the Fukui Matrix and Function for Systems with (Quasi-)Degenerate States. Journal of Chemical Theory and Computation, 2014, 10, 202-210.	5.3	53
43	High-Speed Calculation of AIM Charges through the Electronegativity Equalization Method. Journal of Physical Chemistry A, 2004, 108, 10359-10366.	2.5	52
44	Aromaticity in linear polyacenes: Generalized population analysis and molecular quantum similarity approach. Journal of Computational Chemistry, 2007, 28, 152-160.	3.3	51
45	Multicenter Bond Indices As a New Means for the Quantitative Characterization of Homoaromaticity. Journal of Physical Chemistry A, 2005, 109, 6606-6609.	2.5	50
46	Exact ionization potentials from wavefunction asymptotics: The extended Koopmansâ€™ theorem, revisited. Journal of Chemical Physics, 2009, 130, 194104.	3.0	48
47	Atomic Charges and the Electrostatic Potential Are Ill-Defined in Degenerate Ground States. Journal of Chemical Theory and Computation, 2013, 9, 4779-4788.	5.3	48
48	Determination of the Absolute Configuration of Threeas-Hydrindacene Compounds by Vibrational Circular Dichroism. Journal of Organic Chemistry, 2005, 70, 9103-9114.	3.2	47
49	Intermolecular Association of Tetrahydrofuran-2-carboxylic Acid in Solution:Â A Vibrational Circular Dichroism Study. Journal of Physical Chemistry A, 2006, 110, 10191-10200.	2.5	47
50	Comparative Study of Aromaticity in Tetraoxa[8]circulenes. Journal of Physical Chemistry A, 2012, 116, 9421-9430.	2.5	46
51	Simple and inexpensive perturbative correction schemes for antisymmetric products of nonorthogonal geminals. Physical Chemistry Chemical Physics, 2014, 16, 5061.	2.8	46
52	Variational Optimization of the Second-Order Density Matrix Corresponding to a Seniority-Zero Configuration Interaction Wave Function. Journal of Chemical Theory and Computation, 2015, 11, 4064-4076.	5.3	46
53	Quantum Similarity Superposition Algorithm (QSSA):â€‰ A Consistent Scheme for Molecular Alignment and Molecular Similarity Based on Quantum Chemistry. Journal of Chemical Information and Density functional theory study of La<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Ce<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mml:	2.8	44
54		3.2	43

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55	Ab initio conformational analysis of ethylene glycol and 1,3-propanediol. Computational and Theoretical Chemistry, 1995, 357, 19-32.	1.5	42
56	Similarity and Chirality:Â Quantum Chemical Study of Dissimilarity of Enantiomers. Journal of Physical Chemistry A, 2003, 107, 11120-11127.	2.5	42
57	Incorrect diatomic dissociation in variational reduced density matrix theory arises from the flawed description of fractionally charged atoms. Physical Chemistry Chemical Physics, 2009, 11, 5558.	2.8	42
58	The Significance of Parameters in Charge Equilibration Models. Journal of Chemical Theory and Computation, 2011, 7, 1750-1764.	5.3	42
59	Subsystem constraints in variational second order density matrix optimization: Curing the dissociative behavior. Journal of Chemical Physics, 2010, 132, 114113.	3.0	41
60	Covalency and Ionicity Do Not Oppose Each Otherâ€"Relationship Between Siâ^'O Bond Character and Basicity of Siloxanes. Chemistry - A European Journal, 2018, 24, 15275-15286.	3.3	40
61	Multicenter delocalization indices vs. properties of the electron density at ring critical points: A study on polycyclic aromatic hydrocarbons. Chemical Physics Letters, 2006, 433, 5-9.	2.6	38
62	Bonding Study in All-Metal Clusters Containing Al4Units. Journal of Physical Chemistry A, 2007, 111, 11885-11893.	2.5	38
63	Influence of Atoms-in-Molecules Methods on Shared-Electron Distribution Indices and Domain-Averaged Fermi Holes^{â€}. Journal of Physical Chemistry A, 2010, 114, 8754-8763.	2.5	38
64	When is the Fukui Function Not Normalized? The Danger of Inconsistent Energy Interpolation Models in Density Functional Theory. Journal of Chemical Theory and Computation, 2016, 12, 5777-5787.	5.3	38
65	Quality of Approximate Electron Densities and Internal Consistency of Molecular Alignment Algorithms in Molecular Quantum Similarity. Journal of Chemical Information and Computer Sciences, 2003, 43, 1208-1217.	2.8	36
66	Performance of 3Dâ€spaceâ€based atomsâ€inâ€molecules methods for electronic delocalization aromaticity indices. Journal of Computational Chemistry, 2011, 32, 386-395.	3.3	36
67	A hybrid configuration interaction treatment based on seniority number and excitation schemes. Journal of Chemical Physics, 2014, 141, 244118.	3.0	36
68	Tetravalent Doping of <scp><scp>CeO</scp></scp>₂: The Impact of Valence Electron Character on Group IV Dopant Influence. Journal of the American Ceramic Society, 2014, 97, 258-266.	3.8	36
69	Molecular quantum similarity of enantiomers of amino acids: a case study. Computational and Theoretical Chemistry, 2005, 727, 49-56.	1.5	35
70	A new computer program for QSAR-analysis: ARTE-QSAR. Journal of Computational Chemistry, 2007, 28, 1924-1928.	3.3	35
71	Molecular Dynamics and Umbrella Sampling Study of Stabilizing Factors in Cyclic Peptide-Based Nanotubes. Journal of Physical Chemistry B, 2012, 116, 9922-9933.	2.6	35
72	A selected ion flow tube study of the reactions of H3O+, NO+ and O2+ with a series of sesquiterpenes. International Journal of Mass Spectrometry, 2008, 272, 137-148.	1.5	34

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73	Theoretical studies on the transport mechanism of 5-fluorouracil through cyclic peptide based nanotubes. Physical Chemistry Chemical Physics, 2013, 15, 1260-1270.	2.8	32
74	Axially chiral BODIPYs. Chemical Communications, 2014, 50, 4714-4716.	4.1	32
75	A DFT conformational analysis and VCD study on methyl tetrahydrofuran-2-carboxylate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 67, 402-411.	3.9	31
76	How Does Aromaticity Rule the Thermodynamic Stability of Hydroporphyrins?. Chemistry - A European Journal, 2011, 17, 3274-3286.	3.3	31
77	On the Determination of the Stereochemistry of Semisynthetic Natural Product Analogues using Chiroptical Spectroscopy: Desulfurization of Epidithiodioxopiperazine Fungal Metabolites. Chemistry - A European Journal, 2011, 17, 11868-11875.	3.3	31
78	Molecular Quantum Similarity Matrix Based Clustering of Molecules Using Dendrograms. Journal of Chemical Information and Computer Sciences, 2003, 43, 170-177.	2.8	30
79	A General Procedure to Obtain Quantum Mechanical Charge and Bond Order Molecular Parameters. Journal of Mathematical Chemistry, 2004, 36, 201-210.	1.5	30
80	Determination of absolute configuration via vibrational circular dichroism. Drug Discovery Today: Technologies, 2004, 1, 269-275.	4.0	30
81	Coulomb and Overlap Self-Similarities:Â A Comparative Selectivity Analysis of Structureâ^'Function Relationships for Auxinâ^'like Molecules. Journal of Chemical Information and Modeling, 2006, 46, 1751-1762.	5.4	30
82	Multidimensionality of delocalization indices and nucleusâ€independent chemical shifts in polycyclic aromatic hydrocarbons II: Proof of further nonlocality. Journal of Computational Chemistry, 2010, 31, 2286-2293.	3.3	30
83	Chemical verification of variational second-order density matrix based potential energy surfaces for the N2 isoelectronic series. Journal of Chemical Physics, 2010, 132, 114112.	3.0	30
84	Local aromaticity of the five-membered rings in acenaphthylene derivatives. Physical Chemistry Chemical Physics, 2012, 14, 14067.	2.8	30
85	Vibrational Circular Dichroism versus Optical Rotation Dispersion and Electronic Circular Dichroism for diastereomers: the stereochemistry of 3-(1â€²-hydroxyethyl)-1-(3â€²-phenylpropanoyl)-azetidin-2-one. Physical Chemistry Chemical Physics, 2012, 14, 8562.	2.8	30
86	Tribenzotriquinacene Receptors for C₆₀â€...Fullerene Rotors: Towards C₃ Symmetrical Chiral Stators for Unidirectionally Operating Nanoratchets. Chemistry - A European Journal, 2014, 20, 9100-9110.	3.3	30
87	Fast Calculation of Quantum Chemical Molecular Descriptors from the Electronegativity Equalization Method. Journal of Chemical Information and Computer Sciences, 2003, 43, 422-428.	2.8	29
88	A selected ion flow tube study of the reactions of H3O+, NO+ and O2+ with some oxygenated biogenic volatile organic compounds. International Journal of Mass Spectrometry, 2005, 247, 1-9.	1.5	29
89	Molecular quantum similarity using conceptual DFT descriptors. Journal of Chemical Sciences, 2005, 117, 425-435.	1.5	29
90	A primalâ€“dual semidefinite programming algorithm tailored to the variational determination of the two-body density matrix. Computer Physics Communications, 2011, 182, 1235-1244.	7.5	29

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91	Tuning of CeO2 buffer layers for coated superconductors through doping. Applied Surface Science, 2012, 260, 32-35.	6.1	29
92	Interplay between Hydrogen-Bond Formation and Multicenter Ï€-Electron Delocalization: Intramolecular Hydrogen Bonds. Journal of Physical Chemistry A, 2008, 112, 10689-10696.	2.5	28
93	Reply to â€˜comment on â€œextending Hirshfeldâ€¦ to bulk and periodic materialsâ€â€™. Journal of Computational Chemistry, 2013, 34, 422-427.	3.3	28
94	Interpreting the behavior of the by resolving in orbitals, sign, and positions. Journal of Computational Chemistry, 2018, 39, 511-519.	3.3	28
95	Three-Dimensional Fully Ï€-Conjugated Macrocycles: When 3D-Aromatic and When 2D-Aromatic-in-3D?. Journal of the American Chemical Society, 2022, 144, 8560-8575.	13.7	28
96	Aromaticity and Homoaromaticity in Methano[10]annulenes. Journal of Organic Chemistry, 2007, 72, 76-85.	3.2	27
97	The pseudo-Ï€ method examined for the computation of multicenter aromaticity indices. Journal of Mathematical Chemistry, 2008, 43, 111-118.	1.5	27
98	Richardsonâ€“Gaudin mean-field for strong correlation in quantum chemistry. Journal of Chemical Physics, 2020, 153, 104110.	3.0	27
99	Aromaticity in cyclic alkali clusters. Physical Chemistry Chemical Physics, 2008, 10, 2461.	2.8	26
100	Influence of electron correlation and degeneracy on the Fukui matrix and extension of frontier molecular orbital theory to correlated quantum chemical methods. Physical Chemistry Chemical Physics, 2012, 14, 2408.	2.8	25
101	Direct variational determination of the two-electron reduced density matrix for doubly occupied-configuration-interaction wave functions: The influence of three-index N-representability conditions. Journal of Chemical Physics, 2018, 148, 024105.	3.0	25
102	A selected ion flow tube study of the reactions of H3O+, NO+ and O2+ with a series of C5, C6 and C8 unsaturated biogenic alcohols. International Journal of Mass Spectrometry, 2007, 263, 127-136.	1.5	24
103	Interplay Between Hydrogen Bond Formation and Multicenter Ï€-Electron Delocalization: Intermolecular Hydrogen Bonds. Journal of Physical Chemistry A, 2008, 112, 7898-7904.	2.5	24
104	3D QSAR based on conceptual DFT molecular fields: Antituberculotic activity. Computational and Theoretical Chemistry, 2010, 943, 83-89.	1.5	24
105	Polynomial scaling approximations and dynamic correlation corrections to doubly occupied configuration interaction wave functions. Journal of Chemical Physics, 2015, 143, 104106.	3.0	24
106	A combined Raman optical activity and vibrational circular dichroism study on artemisinin-type products. Physical Chemistry Chemical Physics, 2020, 22, 18014-18024.	2.8	24
107	Prediction of bloodâ€“brain partitioning: A model based on ab initio calculated quantum chemical descriptors. Journal of Molecular Graphics and Modelling, 2008, 26, 1223-1236.	2.4	23
108	Strength by Joining Methods: Combining Synthesis with NMR, IR, and Vibrational Circular Dichroism Spectroscopy for the Determination of the Relative Configuration in Hemicalide. Chemistry - A European Journal, 2014, 20, 17385-17394.	3.3	23

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109	Study of Molecular Quantum Similarity of Enantiomers of Amino Acids. Journal of Physical Chemistry A, 2006, 110, 5114-5120.	2.5	22
110	Quantifying the conceptual problems associated with the isotropic NICS through analyses of its underlying density. Physical Chemistry Chemical Physics, 2019, 21, 3145-3153.	2.8	22
111	Partitioning of the molecular density matrix over atoms and bonds. Journal of Chemical Physics, 2010, 132, 164111.	3.0	21
112	A selfâ€consistent Hirshfeld method for the atom in the molecule based on minimization of information loss. Journal of Computational Chemistry, 2011, 32, 1561-1567.	3.3	21
113	Ab initio conformational analysis of the chelating bidentate ligands ethylenediamine and 1,3-propanediamine. Computational and Theoretical Chemistry, 1995, 339, 1-14.	1.5	20
114	Ab initio and molecular mechanics study of 1,2-dimethoxyethane and 12-crown-4. Computational and Theoretical Chemistry, 1999, 467, 211-222.	1.5	20
115	Unrevealed structural requirements for auxin-like molecules by theoretical and experimental evidences. Phytochemistry, 2007, 68, 237-250.	2.9	20
116	Aromaticity in all-metal annular systems: the counter-ion effect. Physical Chemistry Chemical Physics, 2011, 13, 14865.	2.8	20
117	Structure and stability of cyclic peptide based nanotubes: a molecular dynamics study of the influence of amino acid composition. Physical Chemistry Chemical Physics, 2012, 14, 15135.	2.8	20
118	Algebraic relationships between conceptual DFT quantities and the electronegativity equalization hardness matrix. Chemical Physics Letters, 2002, 364, 357-362.	2.6	19
119	Multicenter Bonding in Carbocations with Tetracoordinate Protons. Journal of Physical Chemistry A, 2006, 110, 3785-3789.	2.5	19
120	Statistical Validation of Absolute Configuration Assignment in Vibrational Optical Activity. Journal of Chemical Theory and Computation, 2013, 9, 5504-5512.	5.3	19
121	Strategies for extending geminal-based wavefunctions: Open shells and beyond. Computational and Theoretical Chemistry, 2017, 1116, 207-219.	2.5	19
122	Absolute configuration and biological profile of pyrazoline enantiomers as MAO inhibitory activity. Chirality, 2019, 31, 21-33.	2.6	19
123	Evidence from current-density mapping for Ïƒ-delocalisation in the aromatic hexaiodobenzene cation. Tetrahedron Letters, 2008, 49, 1421-1424.	1.4	18
124	Conceptual DFT propertiesâ€based 3D QSAR: Analysis of inhibitors of the nicotine metabolizing CYP2A6 enzyme. Journal of Computational Chemistry, 2009, 30, 1749-1757.	3.3	18
125	Ring Currents in Polycyclic Sodium Clusters. Journal of Physical Chemistry A, 2011, 115, 12493-12502.	2.5	18
126	Enantio- and diastereoselective palladium catalysed arylative and vinylative allene carbocyclisation cascades. Chemical Communications, 2013, 49, 5265.	4.1	18

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127	The effect of protein backbone hydration on the amide vibrations in Raman and Raman optical activity spectra. Physical Chemistry Chemical Physics, 2019, 21, 1988-2005.	2.8	18
128	Study of the deposition and Raman and XPS characterization of a metal ion tetrasulphonated phthalocyanine layer at gold surfaces: density functional theory calculations to model the vibrational spectra. Electrochemistry Communications, 2005, 7, 87-96.	4.7	17
129	QSAR analysis of salicylamide isosteres with the use of quantum chemical molecular descriptors. European Journal of Medicinal Chemistry, 2009, 44, 869-876.	5.5	17
130	Mechanistic and Chiroptical Studies on the Desulfurization of Epidithiodioxopiperazines Reveal Universal Retention of Configuration at the Bridgehead Carbon Atoms. Journal of Organic Chemistry, 2013, 78, 11646-11655.	3.2	17
131	Stereochemistry of the Brivaracetam Diastereoisomers. Chirality, 2016, 28, 215-225.	2.6	17
132	The effect of hydrogen bond strength on emission properties in 2-(2â€²-hydroxyphenyl)imidazo[1,2-a]pyridines. Journal of Photochemistry and Photobiology A: Chemistry, 2016, 314, 198-213.	3.9	17
133	Toward an Alternative Hardness Kernel Matrix Structure in the Electronegativity Equalization Method (EEM). Journal of Chemical Information and Modeling, 2006, 46, 1657-1665.	5.4	16
134	An Atom Counting QSPR Protocol. QSAR and Combinatorial Science, 2008, 27, 208-230.	1.4	16
135	Deriving the Hirshfeld partitioning using distance metrics. Journal of Chemical Physics, 2014, 141, 094103.	3.0	16
136	Performance of Shannon-entropy compacted N-electron wave functions for configuration interaction methods. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	16
137	Triplet state homoaromaticity: concept, computational validation and experimental relevance. Chemical Science, 2018, 9, 3165-3176.	7.4	16
138	The close relation between cyclic delocalization, energy effects of cycles and aromaticity. Collection of Czechoslovak Chemical Communications, 2009, 74, 147-166.	1.0	16
139	Substituent effects in 1,4-disubstituted benzene and cyclohexadiene: Olefinic vs aromatic electron shift pathway of the substituent effect. Computational and Theoretical Chemistry, 2012, 984, 36-42.	2.5	15
140	Electron Momentum Spectroscopy of 1-Butene: A Theoretical Analysis Using Molecular Dynamics and Molecular Quantum Similarity. Journal of Physical Chemistry A, 2013, 117, 8388-8398.	2.5	15
141	Extended random phase approximation method for atomic excitation energies from correlated and variationally optimized second-order density matrices. Computational and Theoretical Chemistry, 2013, 1003, 50-54.	2.5	15
142	A problematic issue for atoms in molecules: Impact of (quasi-)degenerate states on Quantum Theory Atoms in Molecules and Hirshfeld-I properties. Computational and Theoretical Chemistry, 2015, 1053, 106-111.	2.5	15
143	Ring Currents in Benzoâ€•and Benzocyclobutadienoâ€Annelated Biphenylene Derivatives. ChemPhysChem, 2015, 16, 216-222.	2.1	15
144	Exploring the role of the 3-centerâ€“4-electron bond in hypervalent Î»‹sup›3‹/sup›-iodanes using the methodology of domain averaged Fermi holes. Physical Chemistry Chemical Physics, 2016, 18, 846-856.	2.8	15

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145	Near-exact treatment of seniority-zero ground and excited states with a Richardsonâ€“Gaudin mean-field. Journal of Chemical Physics, 2022, 156, .	3.0	15
146	Variational second order density matrix study of $mathrm{F_3^-}$: Importance of subspace constraints for size-consistency. Journal of Chemical Physics, 2011, 134, 054115.	3.0	14
147	Striking a Compromise: Polar Functional Group Tolerance versus Insertion Barrier Height for Olefin Polymerization Catalysts. Organometallics, 2012, 31, 6022-6031.	2.3	14
148	Bond fukui indices: Comparison of frozen molecular orbital and finite differences through mulliken populations. Journal of Computational Chemistry, 2013, 34, 2421-2429.	3.3	14
149	Study of ion/molecule reactions of atmospherically important negative ions with methane sulfonic acid. International Journal of Mass Spectrometry, 2002, 221, 209-218.	1.5	13
150	Role of solution conformation and flexibility of short peptide ligands that bind to the p56lck SH2 domain. Bioorganic and Medicinal Chemistry, 2003, 11, 941-949.	3.0	13
151	Stockholder projector analysis: A Hilbert-space partitioning of the molecular one-electron density matrix with orthogonal projectors. Journal of Chemical Physics, 2012, 136, 014107.	3.0	13
152	Aromaticity of Closed-Shell Charged Polybenzenoid Hydrocarbons. Journal of Physical Chemistry A, 2013, 117, 4679-4687.	2.5	13
153	Can the electronegativity equalization method predict spectroscopic properties?. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 76-80.	3.9	13
154	Atom and Bond Fukui Functions and Matrices: A Hirshfeldâ€Ⅰ Atomsâ€inâ€Molecule Approach. ChemPhysChem, 2016, 17, 2881-2889.	2.1	13
155	Vibrational circular dichroism DFT study on bicyclo[3.3.0]octane derivatives. Tetrahedron: Asymmetry, 2006, 17, 3203-3218.	1.8	12
156	On induced current density in the perylene/bisanthrene homologous series. Chemical Physics Letters, 2012, 552, 151-155.	2.6	12
157	Conformational Analysis of [12]aneN4(1,4,7,10-Tetraazacyclododecane) and [14]aneN4(1,4,8,11-Tetraazacyclotetradecane) Using Molecular Mechanics and ab Initio Methods. Journal of Physical Chemistry A, 2000, 104, 11801-11809.	2.5	11
158	Structureâ€“activity analysis on ecdysteroids: A structural and quantum chemical approach based on two biological systems. Computational and Theoretical Chemistry, 2006, 758, 263-274.	1.5	11
159	Alternative Kullbackâ€“Leibler Information Entropy for Enantiomers. Journal of Physical Chemistry A, 2010, 114, 640-645.	2.5	11
160	Considerations on describing non-singlet spin states in variational second order density matrix methods. Journal of Chemical Physics, 2012, 136, 014110.	3.0	11
161	Heterotrimetallic compounds containing Moâ€“Mâ€“Li [M = K, Rb and Cs] clusters: synthesis, structure, bonding, aromaticity and theoretical investigations of Li2M2 [M = K and Rb] and Cs4 rings. Physical Chemistry Chemical Physics, 2012, 14, 15579.	2.8	11
162	Self-consistent methods constrained to a fixed number of particles in a given fragment and its relation to the electronegativity equalization method. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	11

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