

Patrick Bultinck

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/8505603/publications.pdf>

Version: 2024-02-01

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	Uncovering Clar's aromatic sextet rule in the Hubbard model using Maximum Probability Domain Partitions. <i>Journal of Computational Chemistry</i> , 2022, 43, 457-464.	3.3	3
2	Constrained iterative Hirshfeld charges: A variational approach. <i>Journal of Chemical Physics</i> , 2022, 156, .	3.0	2
3	Three-Dimensional Fully π -Conjugated Macrocycles: When 3D-Aromatic and When 2D-Aromatic-in-3D?. <i>Journal of the American Chemical Society</i> , 2022, 144, 8560-8575.	13.7	28
4	Near-exact treatment of seniority-zero ground and excited states with a Richardson-Gaudin mean-field. <i>Journal of Chemical Physics</i> , 2022, 156, .	3.0	15
5	Analyzing the Behavior of Spin Phases in External Magnetic Fields by Means of Spin-Constrained States. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3364-3376.	5.3	2
6	Exploring machine learning methods for absolute configuration determination with vibrational circular dichroism. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 19781-19789.	2.8	7
7	GQCP: The Ghent Quantum Chemistry Package. <i>Journal of Chemical Physics</i> , 2021, 155, 084802.	3.0	11
8	Quantifying Delocalization and Static Correlation Errors by Imposing (Spin)Population Redistributions through Constraints on Atomic Domains. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6808-6818.	5.3	4
9	Hierarchies of quantum chemical descriptors induced by statistical analyses of domain occupation number operators. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2020, 10, e1456.	14.6	4
10	Richardson-Gaudin mean-field for strong correlation in quantum chemistry. <i>Journal of Chemical Physics</i> , 2020, 153, 104110.	3.0	27
11	A combined Raman optical activity and vibrational circular dichroism study on artemisinin-type products. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 18014-18024.	2.8	24
12	CFA-18: a homochiral metal-organic framework (MOF) constructed from rigid enantiopure bistriazolate linker molecules. <i>Dalton Transactions</i> , 2020, 49, 15758-15768.	3.3	7
13	Comparative Study of the Vibrational Optical Activity Techniques in Structure Elucidation: The Case of Galantamine. <i>ACS Omega</i> , 2019, 4, 14133-14139.	3.5	9
14	Quantifying the conceptual problems associated with the isotropic NICS through analyses of its underlying density. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 3145-3153.	2.8	22
15	The effect of protein backbone hydration on the amide vibrations in Raman and Raman optical activity spectra. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 1988-2005.	2.8	18
16	Absolute configuration and biological profile of pyrazoline enantiomers as MAO inhibitory activity. <i>Chirality</i> , 2019, 31, 21-33.	2.6	19
17	A simple algorithm for the Kohn-Sham inversion problem applicable to general target densities. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	1.4	11
18	Triplet state homoaromaticity: concept, computational validation and experimental relevance. <i>Chemical Science</i> , 2018, 9, 3165-3176.	7.4	16

#	ARTICLE	IF	CITATIONS
19	Method for making 2-electron response reduced density matrices approximately N -representable. <i>Journal of Chemical Physics</i> , 2018, 148, 084104.	3.0	6
20	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. <i>Journal of Chemical Physics</i> , 2018, 148, 024105.	3.0	25
21	Interpreting the behavior of the by resolving in orbitals, sign, and positions. <i>Journal of Computational Chemistry</i> , 2018, 39, 511-519.	3.3	28
22	Information-Theoretic Approaches to Atoms-in-Molecules: Hirshfeld Family of Partitioning Schemes. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4219-4245.	2.5	97
23	Conformational Disorder and Dynamics of Proteins Sensed by Raman Optical Activity. <i>ACS Omega</i> , 2018, 3, 12944-12955.	3.5	11
24	The influence of correlation on (de)localization indices from a valence bond perspective. <i>Journal of Molecular Modeling</i> , 2018, 24, 275.	1.8	3
25	Covalency and Ionicity Do Not Oppose Each Other—Relationship Between σ Bond Character and Basicity of Siloxanes. <i>Chemistry - A European Journal</i> , 2018, 24, 15275-15286.	3.3	40
26	Strategies for extending geminal-based wavefunctions: Open shells and beyond. <i>Computational and Theoretical Chemistry</i> , 2017, 1116, 207-219.	2.5	19
27	Analysis of molecular and (di)atomic dual-descriptor functions and matrices. <i>Journal of Molecular Modeling</i> , 2017, 23, 185.	1.8	0
28	Model-averaging of ab initio spectra for the absolute configuration assignment via vibrational circular dichroism. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 28028-28036.	2.8	10
29	Fractional nuclear charge approach to isolated anion densities for Hirshfeld partitioning methods. <i>Journal of Molecular Modeling</i> , 2017, 23, 348.	1.8	5
30	Stereochemistry of the Brivaracetam Diastereoisomers. <i>Chirality</i> , 2016, 28, 215-225.	2.6	17
31	Performance of Shannon-entropy compacted N -electron wave functions for configuration interaction methods. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	1.4	16
32	Atom and Bond Fukui Functions and Matrices: A Hirshfeld—Atoms—Molecule Approach. <i>ChemPhysChem</i> , 2016, 17, 2881-2889.	2.1	13
33	4th International Conference on Chemical Bonding. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9353-9356.	2.5	1
34	When is the Fukui Function Not Normalized? The Danger of Inconsistent Energy Interpolation Models in Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5777-5787.	5.3	38
35	Addendum to “More insight in multiple bonding with valence bond theory” [Comput. Theor. Chem. 1053 (2015) 180–188]. <i>Computational and Theoretical Chemistry</i> , 2016, 1079, 70.	2.5	0
36	Maximum probability domains for Hubbard models. <i>Molecular Physics</i> , 2016, 114, 1392-1405.	1.7	10

#	ARTICLE	IF	CITATIONS
37	Exploring the role of the 3-center-4-electron bond in hypervalent I^{III} -iodanes using the methodology of domain averaged Fermi holes. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 846-856.	2.8	15
38	Can the current density map topology be extracted from the nucleus independent chemical shifts?. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11746-11755.	2.8	61
39	The effect of hydrogen bond strength on emission properties in 2-(2-hydroxyphenyl)imidazo[1,2-a]pyridines. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2016, 314, 198-213.	3.9	17
40	Three-dimensional networks containing rectangular Sr_4 and Ba_4 units: Synthesis, structure, bonding, and potential application for Ne gas separation. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 1501-1510.	2.0	6
41	Elucidation of the absolute configuration of rhizopine by chiral supercritical fluid chromatography and vibrational circular dichroism. <i>Journal of Separation Science</i> , 2015, 38, 2545-2550.	2.5	10
42	Chiroptical Studies on Brevianamide B: Vibrational and Electronic Circular Dichroism Confronted. <i>Journal of Organic Chemistry</i> , 2015, 80, 3359-3367.	3.2	7
43	A problematic issue for atoms in molecules: Impact of (quasi-)degenerate states on Quantum Theory Atoms in Molecules and Hirshfeld-I properties. <i>Computational and Theoretical Chemistry</i> , 2015, 1053, 106-111.	2.5	15
44	FA-SIFT study of the reactions of $\text{H}_3\text{O}^+(\text{H}_2\text{O})$ ($n = 0, 1, 2$), NO^+ and O_2^+ with the terpenoid aldehydes citral, citronellal and myrtenal and their alcohol analogues. <i>International Journal of Mass Spectrometry</i> , 2015, 379, 52-59.	1.5	5
45	Variational Optimization of the Second-Order Density Matrix Corresponding to a Seniority-Zero Configuration Interaction Wave Function. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4064-4076.	5.3	46
46	Polynomial scaling approximations and dynamic correlation corrections to doubly occupied configuration interaction wave functions. <i>Journal of Chemical Physics</i> , 2015, 143, 104106.	3.0	24
47	More insight in multiple bonding with valence bond theory. <i>Computational and Theoretical Chemistry</i> , 2015, 1053, 180-188.	2.5	6
48	Can the electronegativity equalization method predict spectroscopic properties?. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 76-80.	3.9	13
49	Ring Currents in Benzo- and Benzocyclobutadieno-Annulated Biphenylene Derivatives. <i>ChemPhysChem</i> , 2015, 16, 216-222.	2.1	15
50	Six questions on topology in theoretical chemistry. <i>Computational and Theoretical Chemistry</i> , 2015, 1053, 2-16.	2.5	99
51	Projected seniority-two orbital optimization of the antisymmetric product of one-reference orbital geminal. <i>Journal of Chemical Physics</i> , 2014, 140, 214114.	3.0	68
52	Deriving the Hirshfeld partitioning using distance metrics. <i>Journal of Chemical Physics</i> , 2014, 141, 094103.	3.0	16
53	A hybrid configuration interaction treatment based on seniority number and excitation schemes. <i>Journal of Chemical Physics</i> , 2014, 141, 244118.	3.0	36
54	Axially chiral BODIPYs. <i>Chemical Communications</i> , 2014, 50, 4714-4716.	4.1	32

#	ARTICLE	IF	CITATIONS
55	Efficient description of strongly correlated electrons with mean-field cost. <i>Physical Review B</i> , 2014, 89, .	3.2	95
56	How to Compute the Fukui Matrix and Function for Systems with (Quasi-)Degenerate States. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 202-210.	5.3	53
57	The influence of orbital rotation on the energy of closed-shell wavefunctions. <i>Molecular Physics</i> , 2014, 112, 853-862.	1.7	84
58	Tetravalent Doping of CeO_2 : The Impact of Valence Electron Character on Group IV Dopant Influence. <i>Journal of the American Ceramic Society</i> , 2014, 97, 258-266.	3.8	36
59	Strength by Joining Methods: Combining Synthesis with NMR, IR, and Vibrational Circular Dichroism Spectroscopy for the Determination of the Relative Configuration in Hemicalide. <i>Chemistry - A European Journal</i> , 2014, 20, 17385-17394.	3.3	23
60	Aliovalent doping of CeO_2 : DFT study of oxidation state and vacancy effects. <i>Journal of Materials Chemistry A</i> , 2014, 2, 13723-13737.	10.3	93
61	Simple and inexpensive perturbative correction schemes for antisymmetric products of nonorthogonal geminals. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 5061.	2.8	46
62	Nonvariational Orbital Optimization Techniques for the AP1roG Wave Function. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4873-4882.	5.3	59
63	Tribenzotriquinacene Receptors for C_{60} ...Fullerene Rotors: Towards C_{30} Symmetrical Chiral Stators for Unidirectionally Operating Nanoratchets. <i>Chemistry - A European Journal</i> , 2014, 20, 9100-9110.	3.3	30
64	Self-consistent methods constrained to a fixed number of particles in a given fragment and its relation to the electronegativity equalization method. <i>Highlights in Theoretical Chemistry</i> , 2014, , 27-33.	0.0	0
65	Enantio- and diastereoselective palladium catalysed arylative and vinylative allene carbocyclisation cascades. <i>Chemical Communications</i> , 2013, 49, 5265.	4.1	18
66	Performance of DFT Methods in Momentum Space: Quantum Similarity Measures versus Moments of Momentum. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3908-3916.	5.3	0
67	Bond fukui indices: Comparison of frozen molecular orbital and finite differences through mulliken populations. <i>Journal of Computational Chemistry</i> , 2013, 34, 2421-2429.	3.3	14
68	Removal of the Pyridine Directing Group from $\hat{1}\pm$ -Substituted N -(Pyridin-2-yl)piperidines Obtained via Directed Ru-Catalyzed $\text{sp}^3\text{C-H}$ Functionalization. <i>Journal of Organic Chemistry</i> , 2013, 78, 9803-9814.	3.2	53
69	Electron Momentum Spectroscopy of 1-Butene: A Theoretical Analysis Using Molecular Dynamics and Molecular Quantum Similarity. <i>Journal of Physical Chemistry A</i> , 2013, 117, 8388-8398.	2.5	15
70	Mechanistic and Chiroptical Studies on the Desulfurization of Epidithiodioxopiperazines Reveal Universal Retention of Configuration at the Bridgehead Carbon Atoms. <i>Journal of Organic Chemistry</i> , 2013, 78, 11646-11655.	3.2	17
71	Atomic Charges and the Electrostatic Potential Are Ill-Defined in Degenerate Ground States. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4779-4788.	5.3	48
72	Extended random phase approximation method for atomic excitation energies from correlated and variationally optimized second-order density matrices. <i>Computational and Theoretical Chemistry</i> , 2013, 1003, 50-54.	2.5	15

#	ARTICLE	IF	CITATIONS
73	Reply to "comment on "extending Hirshfeld" to bulk and periodic materials". Journal of Computational Chemistry, 2013, 34, 422-427.	3.3	28
74	Statistical Validation of Absolute Configuration Assignment in Vibrational Optical Activity. Journal of Chemical Theory and Computation, 2013, 9, 5504-5512.	5.3	19
75	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
76	Aromaticity of Closed-Shell Charged Polybenzenoid Hydrocarbons. Journal of Physical Chemistry A, 2013, 117, 4679-4687.	2.5	13
77	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
78	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
79	Synthesis of the Natural Product Building Block 5-(3-bromophenyl)-4-hydroxy-5-methylhexan-2-one and its Chiral Characterization by Using Chiroptical Spectroscopy. ChemPhysChem, 2013, 14, 3255-3262.	2.1	2
80	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
81	Extending Hirshfeld" to bulk and periodic materials. Journal of Computational Chemistry, 2013, 34, 405-417.	3.3	72
82	Considerations on describing non-singlet spin states in variational second order density matrix methods. Journal of Chemical Physics, 2012, 136, 014110.	3.0	11
83	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
84	Heterotrimetallic compounds containing Mo-M-Li [M = K, Rb and Cs] clusters: synthesis, structure, bonding, aromaticity and theoretical investigations of Li ₂ M ₂ [M = K and Rb] and Cs ₄ rings. Physical Chemistry Chemical Physics, 2012, 14, 15579.	2.8	11
85	On induced current density in the perylene/bisanthrene homologous series. Chemical Physics Letters, 2012, 552, 151-155.	2.6	12
86	Local aromaticity of the five-membered rings in acenaphthylene derivatives. Physical Chemistry Chemical Physics, 2012, 14, 14067.	2.8	30
87	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
88	Striking a Compromise: Polar Functional Group Tolerance versus Insertion Barrier Height for Olefin Polymerization Catalysts. Organometallics, 2012, 31, 6022-6031.	2.3	14
89	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
90	Vibrational Circular Dichroism versus Optical Rotation Dispersion and Electronic Circular Dichroism for diastereomers: the stereochemistry of 3-(1-hydroxyethyl)-1-(3-phenylpropanoyl)-azetidin-2-one. Physical Chemistry Chemical Physics, 2012, 14, 8562.	2.8	30

#	ARTICLE	IF	CITATIONS
91	Tuning of CeO ₂ buffer layers for coated superconductors through doping. Applied Surface Science, 2012, 260, 32-35.	6.1	29
92	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
93	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
94	Comparative Study of Aromaticity in Tetraoxa[8]circulenes. Journal of Physical Chemistry A, 2012, 116, 9421-9430.	2.5	46
95	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
96	Aromaticity in all-metal annular systems: the counter-ion effect. Physical Chemistry Chemical Physics, 2011, 13, 14865.	2.8	20
97	Ring Currents in Polycyclic Sodium Clusters. Journal of Physical Chemistry A, 2011, 115, 12493-12502. Density functional theory study of La ₂ Ce	2.5	18
98	La ₂ CeO ₂ The Significance of Parameters in Charge Equilibration Models. Journal of Chemical Theory and Computation, 2011, 7, 1750-1764.	3.2	43
99	The Significance of Parameters in Charge Equilibration Models. Journal of Chemical Theory and Computation, 2011, 7, 1750-1764.	5.3	42
100	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
101	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
102	Electron delocalization and aromaticity in low-lying excited states of archetypal organic compounds. Physical Chemistry Chemical Physics, 2011, 13, 20690.	2.8	116
103	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
104	Performance of 3D-based atoms-in-molecules methods for electronic delocalization aromaticity indices. Journal of Computational Chemistry, 2011, 32, 386-395.	3.3	36
105	A self-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
106	Fast density matrix-based partitioning of the energy over the atoms in a molecule consistent with the hirshfeld partitioning of the electron density. Journal of Computational Chemistry, 2011, 32, 3485-3496.	3.3	6
107	How Does Aromaticity Rule the Thermodynamic Stability of Hydroporphyrins?. Chemistry - A European Journal, 2011, 17, 3274-3286.	3.3	31
108	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

#	ARTICLE	IF	CITATIONS
109	Variational density matrix optimization using semidefinite programming. <i>Computer Physics Communications</i> , 2011, 182, 2025-2028.	7.5	1
110	A primal-dual semidefinite programming algorithm tailored to the variational determination of the two-body density matrix. <i>Computer Physics Communications</i> , 2011, 182, 1235-1244.	7.5	29
111	Variational second order density matrix study of F_3^+ : Importance of subspace constraints for size-consistency. <i>Journal of Chemical Physics</i> , 2011, 134, 054115.	3.0	14
112	Communication: Hilbert-space partitioning of the molecular one-electron density matrix with orthogonal projectors. <i>Journal of Chemical Physics</i> , 2010, 133, 231103.	3.0	9
113	Multidimensionality of delocalization indices and nucleus-independent chemical shifts in polycyclic aromatic hydrocarbons II: Proof of further nonlocality. <i>Journal of Computational Chemistry</i> , 2010, 31, 2286-2293.	3.3	30
114	3D QSAR based on conceptual DFT molecular fields: Antituberculous activity. <i>Computational and Theoretical Chemistry</i> , 2010, 943, 83-89.	1.5	24
115	Quantum similarity of isosteres coordinate versus momentum space and influence of alignment. <i>Computational and Theoretical Chemistry</i> , 2010, 943, 183-188.	1.5	9
116	Chemical verification of variational second-order density matrix based potential energy surfaces for the N ₂ isoelectronic series. <i>Journal of Chemical Physics</i> , 2010, 132, 114112.	3.0	30
117	Subsystem constraints in variational second order density matrix optimization: Curing the dissociative behavior. <i>Journal of Chemical Physics</i> , 2010, 132, 114113.	3.0	41
118	Alternative Kullback-Leibler Information Entropy for Enantiomers. <i>Journal of Physical Chemistry A</i> , 2010, 114, 640-645.	2.5	11
119	Influence of Atoms-in-Molecules Methods on Shared-Electron Distribution Indices and Domain-Averaged Fermi Holes. <i>Journal of Physical Chemistry A</i> , 2010, 114, 8754-8763.	2.5	38
120	Partitioning of the molecular density matrix over atoms and bonds. <i>Journal of Chemical Physics</i> , 2010, 132, 164111.	3.0	21
121	Variational determination of the second-order density matrix for the isoelectronic series of beryllium, neon, and silicon. <i>Physical Review A</i> , 2009, 80, .	2.5	59
122	A VCD robust mode analysis of induced chirality: The case of pulegone in chloroform. <i>Chirality</i> , 2009, 21, E287-97.	2.6	63
123	Conceptual DFT properties-based 3D QSAR: Analysis of inhibitors of the nicotine metabolizing CYP2A6 enzyme. <i>Journal of Computational Chemistry</i> , 2009, 30, 1749-1757.	3.3	18
124	QSAR analysis of salicylamide isosteres with the use of quantum chemical molecular descriptors. <i>European Journal of Medicinal Chemistry</i> , 2009, 44, 869-876.	5.5	17
125	Electrostatic Potentials from Self-Consistent Hirshfeld Atomic Charges. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 334-340.	5.3	112
126	Incorrect diatomic dissociation in variational reduced density matrix theory arises from the flawed description of fractionally charged atoms. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 5558.	2.8	42

#	ARTICLE	IF	CITATIONS
127	Exact ionization potentials from wavefunction asymptotics: The extended Koopmans's theorem, revisited. <i>Journal of Chemical Physics</i> , 2009, 130, 194104.	3.0	48
128	Comparison of the Hirshfeld-I and iterated stockholder atoms in molecules schemes. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 3424.	2.8	54
129	The close relation between cyclic delocalization, energy effects of cycles and aromaticity. <i>Collection of Czechoslovak Chemical Communications</i> , 2009, 74, 147-166.	1.0	16
130	Atoms in Molecules and Population Analysis. , 2009, , .		1
131	Molecular Quantum Similarity. , 2009, , .		3
132	A selected ion flow tube study of the reactions of H ₃ O ⁺ , NO ⁺ and O ₂ ⁺ with a series of sesquiterpenes. <i>International Journal of Mass Spectrometry</i> , 2008, 272, 137-148.	1.5	34
133	The pseudo- π method examined for the computation of multicenter aromaticity indices. <i>Journal of Mathematical Chemistry</i> , 2008, 43, 111-118.	1.5	27
134	Mathematical aspects of the LCAO MO first order density function (3): A general localization procedure. <i>Journal of Mathematical Chemistry</i> , 2008, 43, 1069-1075.	1.5	7
135	An Atom Counting QSPR Protocol. <i>QSAR and Combinatorial Science</i> , 2008, 27, 208-230.	1.4	16
136	Correlation of Delocalization Indices and Current-Density Maps in Polycyclic Aromatic Hydrocarbons. <i>Chemistry - A European Journal</i> , 2008, 14, 3093-3099.	3.3	100
137	Multidimensionality of delocalization indices and nucleus independent chemical shifts in polycyclic aromatic hydrocarbons. <i>Journal of Computational Chemistry</i> , 2008, 29, 358-366.	3.3	80
138	Prediction of blood-brain partitioning: A model based on ab initio calculated quantum chemical descriptors. <i>Journal of Molecular Graphics and Modelling</i> , 2008, 26, 1223-1236.	2.4	23
139	Induced solvent chirality: A VCD study of camphor in CDCl ₃ . <i>Chemical Physics Letters</i> , 2008, 450, 426-430.	2.6	60
140	Evidence from current-density mapping for π -delocalisation in the aromatic hexaiodobenzene cation. <i>Tetrahedron Letters</i> , 2008, 49, 1421-1424.	1.4	18
141	Interplay between Hydrogen-Bond Formation and Multicenter π -Electron Delocalization: Intramolecular Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10689-10696.	2.5	28
142	Interplay Between Hydrogen Bond Formation and Multicenter π -Electron Delocalization: Intermolecular Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7898-7904.	2.5	24
143	Solvent effects on IR and VCD spectra of natural products: an experimental and theoretical VCD study of pulegone. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 3498.	2.8	68
144	Aromaticity in cyclic alkali clusters. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 2461.	2.8	26

#	ARTICLE	IF	CITATIONS
145	Bond indices in dihydrogen bonds. <i>Journal of the Brazilian Chemical Society</i> , 2008, 19, .	0.6	3
146	Bonding Study in All-Metal Clusters Containing Al ₄ Units. <i>Journal of Physical Chemistry A</i> , 2007, 111, 11885-11893.	2.5	38
147	Critical analysis and extension of the Hirshfeld atoms in molecules. <i>Journal of Chemical Physics</i> , 2007, 126, 144111.	3.0	577
148	Aromaticity and Homoaromaticity in Methano[10]annulenes. <i>Journal of Organic Chemistry</i> , 2007, 72, 76-85.	3.2	27
149	Critical thoughts on computing atom condensed Fukui functions. <i>Journal of Chemical Physics</i> , 2007, 127, 034102.	3.0	162
150	Comment on "Chemoselectives in Acetalization, Thioacetalization, Oxathioacetalization and Azathioacetalization". <i>Journal of Physical Chemistry A</i> , 2007, 111, 2640-2640.	2.5	3
151	Aromaticity in linear polyacenes: Generalized population analysis and molecular quantum similarity approach. <i>Journal of Computational Chemistry</i> , 2007, 28, 152-160.	3.3	51
152	A new computer program for QSAR-analysis: ARTE-QSAR. <i>Journal of Computational Chemistry</i> , 2007, 28, 1924-1928.	3.3	35
153	Uniqueness and basis set dependence of iterative Hirshfeld charges. <i>Chemical Physics Letters</i> , 2007, 444, 205-208.	2.6	136
154	A selected ion flow tube study of the reactions of H ₃ O ⁺ , NO ⁺ and O ₂ ⁺ with a series of C ₅ , C ₆ and C ₈ unsaturated biogenic alcohols. <i>International Journal of Mass Spectrometry</i> , 2007, 263, 127-136.	1.5	24
155	Unrevealed structural requirements for auxin-like molecules by theoretical and experimental evidences. <i>Phytochemistry</i> , 2007, 68, 237-250.	2.9	20
156	A DFT conformational analysis and VCD study on methyl tetrahydrofuran-2-carboxylate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2007, 67, 402-411.	3.9	31
157	Critical analysis of the local aromaticity concept in polyaromatic hydrocarbons. <i>Faraday Discussions</i> , 2007, 135, 347-365.	3.2	156
158	Electron Delocalization and Aromaticity in Linear Polyacenes: Atoms in Molecules Multicenter Delocalization Index. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7642-7648.	2.5	176
159	Coulomb and Overlap Self-Similarities: A Comparative Selectivity Analysis of Structure-Function Relationships for Auxin-like Molecules. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 1751-1762.	5.4	30
160	Intermolecular Association of Tetrahydrofuran-2-carboxylic Acid in Solution: A Vibrational Circular Dichroism Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 10191-10200.	2.5	47
161	Multicenter Bonding in Carbocations with Tetracoordinate Protons. <i>Journal of Physical Chemistry A</i> , 2006, 110, 3785-3789.	2.5	19
162	Toward an Alternative Hardness Kernel Matrix Structure in the Electronegativity Equalization Method (EEM). <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 1657-1665.	5.4	16

#	ARTICLE	IF	CITATIONS
163	Study of Molecular Quantum Similarity of Enantiomers of Amino Acids. <i>Journal of Physical Chemistry A</i> , 2006, 110, 5114-5120.	2.5	22
164	Multicenter delocalization indices vs. properties of the electron density at ring critical points: A study on polycyclic aromatic hydrocarbons. <i>Chemical Physics Letters</i> , 2006, 433, 5-9.	2.6	38
165	Vibrational circular dichroism DFT study on bicyclo[3.3.0]octane derivatives. <i>Tetrahedron: Asymmetry</i> , 2006, 17, 3203-3218.	1.8	12
166	Structure-activity analysis on ecdysteroids: A structural and quantum chemical approach based on two biological systems. <i>Computational and Theoretical Chemistry</i> , 2006, 758, 263-274.	1.5	11
167	Analyzing Toxicity Through Electrophilicity. <i>Molecular Diversity</i> , 2006, 10, 119-131.	3.9	115
168	Elucidation of the absolute configuration of JNJ-2753292, a CCR2 receptor antagonist, by vibrational circular dichroism analysis of two precursors. <i>Chirality</i> , 2006, 18, 609-620.	2.6	8
169	Local Aromaticity in Polycyclic Aromatic Hydrocarbons: Electron Delocalization versus Magnetic Indices. <i>Chemistry - A European Journal</i> , 2006, 12, 8813-8818.	3.3	90
170	Local Aromaticity in Polycyclic Aromatic Hydrocarbons: Electron Delocalization versus Magnetic Indices. <i>Chemistry - A European Journal</i> , 2006, , .	3.3	1
171	A selected ion flow tube study of the reactions of H ₃ O ⁺ , NO ⁺ and O ₂ ⁺ with some oxygenated biogenic volatile organic compounds. <i>International Journal of Mass Spectrometry</i> , 2005, 247, 1-9.	1.5	29
172	Molecular quantum similarity of enantiomers of amino acids: a case study. <i>Computational and Theoretical Chemistry</i> , 2005, 727, 49-56.	1.5	35
173	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. <i>Electrochemistry Communications</i> , 2005, 7, 87-96.	4.7	17
174	Geometric and electronic similarities between transition structures for electrocyclizations and sigmatropic hydrogen shifts. <i>Theoretical Chemistry Accounts</i> , 2005, 113, 205-211.	1.4	6
175	Molecular quantum similarity using conceptual DFT descriptors. <i>Journal of Chemical Sciences</i> , 2005, 117, 425-435.	1.5	29
176	Multicenter bond indices as a new measure of aromaticity in polycyclic aromatic hydrocarbons. <i>Journal of Physical Organic Chemistry</i> , 2005, 18, 706-718.	1.9	365
177	Molecular Quantum Similarity: Theory and Applications. <i>Reviews in Computational Chemistry</i> , 2005, , 127-207.	1.5	105
178	Multicenter Bond Indices As a New Means for the Quantitative Characterization of Homoaromaticity. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6606-6609.	2.5	50
179	Determination of the Absolute Configuration of Threeas-Hydrindacene Compounds by Vibrational Circular Dichroism. <i>Journal of Organic Chemistry</i> , 2005, 70, 9103-9114.	3.2	47
180	A Mathematical Discussion on Density and Shape Functions, Vector Semispaces and Related Questions. <i>Journal of Mathematical Chemistry</i> , 2004, 36, 191-200.	1.5	61

#	ARTICLE	IF	CITATIONS
181	A General Procedure to Obtain Quantum Mechanical Charge and Bond Order Molecular Parameters. Journal of Mathematical Chemistry, 2004, 36, 201-210.	1.5	30
182	Quantum Mechanical Basis for Mulliken Population Analysis. Journal of Mathematical Chemistry, 2004, 36, 231-239.	1.5	74
183	High-Speed Calculation of AIM Charges through the Electronegativity Equalization Method. Journal of Physical Chemistry A, 2004, 108, 10359-10366.	2.5	52
184	Determination of absolute configuration via vibrational circular dichroism. Drug Discovery Today: Technologies, 2004, 1, 269-275.	4.0	30
185	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
186	Title is missing!. Journal of Mathematical Chemistry, 2003, 34, 75-82.	1.5	4
187	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
188	Quality of Approximate Electron Densities and Internal Consistency of Molecular Alignment Algorithms in Molecular Quantum Similarity.. ChemInform, 2003, 34, no.	0.0	0
189	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
190	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
191	Similarity and Chirality: A Quantum Chemical Study of Dissimilarity of Enantiomers. Journal of Physical Chemistry A, 2003, 107, 11120-11127.	2.5	42
192	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
193	Molecular Quantum Similarity Matrix Based Clustering of Molecules Using Dendrograms. Journal of Chemical Information and Computer Sciences, 2003, 43, 170-177.	2.8	30
194	Negative Fukui functions: New insights based on electronegativity equalization. Journal of Chemical Physics, 2003, 118, 4349-4356.	3.0	114
195	Quantum Similarity Superposition Algorithm (QSSA): A Consistent Scheme for Molecular Alignment and Molecular Similarity Based on Quantum Chemistry. Journal of Chemical Information and Computer Sciences, 2003, 43, 1143-1150.	2.8	44
196	The Electronegativity Equalization Method I: Parametrization and Validation for Atomic Charge Calculations. Journal of Physical Chemistry A, 2002, 106, 7887-7894.	2.5	123
197	The Electronegativity Equalization Method II: Applicability of Different Atomic Charge Schemes. Journal of Physical Chemistry A, 2002, 106, 7895-7901.	2.5	99
198	Generate: A program for 3-D structure generation and conformational analysis of peptides and peptidomimetics. Journal of Computational Chemistry, 2002, 23, 746-754.	3.3	4

#	ARTICLE	IF	CITATIONS
199	Study of ion/molecule reactions of atmospherically important negative ions with methane sulfonic acid. <i>International Journal of Mass Spectrometry</i> , 2002, 221, 209-218.	1.5	13
200	Algebraic relationships between conceptual DFT quantities and the electronegativity equalization hardness matrix. <i>Chemical Physics Letters</i> , 2002, 364, 357-362.	2.6	19
201	Molecular Mechanics and ab Initio Conformational Analysis of 12-Membered and 14-Membered Tetrathia-Crown Ethers. <i>Journal of Physical Chemistry A</i> , 2001, 105, 11266-11275.	2.5	10
202	Theoretical Conformational Analysis of 1,3-Dimethoxypropane and 14-Crown-4: Importance of Stabilizing Intramolecular Interactions. <i>Journal of Physical Chemistry A</i> , 2001, 105, 9203-9210.	2.5	9
203	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. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11801-11809.	2.5	11
204	Ab initio and molecular mechanics study of 1,2-dimethoxyethane and 12-crown-4. <i>Computational and Theoretical Chemistry</i> , 1999, 467, 211-222.	1.5	20
205	Ab initio conformational analysis of 1,3-propanedithiol. <i>Computational and Theoretical Chemistry</i> , 1996, 360, 119-125.	1.5	1
206	Ab initio conformational analysis of the chelating bidentate ligands ethylenediamine and 1,3-propanediamine. <i>Computational and Theoretical Chemistry</i> , 1995, 339, 1-14.	1.5	20
207	Ab initio conformational analysis of ethylene glycol and 1,3-propanediol. <i>Computational and Theoretical Chemistry</i> , 1995, 357, 19-32.	1.5	42
208	Uncovering phase transitions that underpin the flat-planes in the tilted Hubbard model using subsystems and entanglement measures. <i>Journal of Chemical Physics</i> , 0, , .	3.0	2