Peter R SurjÃ¡n

List of Publications by Year
in descending order

173	4,579	109321	128289
papers	citations	35 h-index	60 g-index

183	183	183	2218
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Higher excitations in coupled-cluster theory. Journal of Chemical Physics, 2001, 115, 2945-2954.	3.0	666
2	A general state-selective multireference coupled-cluster algorithm. Journal of Chemical Physics, 2002, 117, 980-990.	3.0	237
3	An observable-based interpretation of electronic wavefunctions: application to â€œhypervalentâ€• molecules. Computational and Theoretical Chemistry, 1992, 255, 9-33.	1.5	137
4	Computing coupled-cluster wave functions with arbitrary excitations. Journal of Chemical Physics, 2000, 113, 1359-1365.	3.0	127
5	An Introduction to the Theory of Geminals. Topics in Current Chemistry, 1999, , 63-88.	4.0	115
6	Monomer geometry relaxation and the basis set superposition error. Chemical Physics Letters, 1992, 191, 497-499.	2.6	113
7	Two-body zeroth order Hamiltonians in multireference perturbation theory: The APSG reference state. Journal of Chemical Physics, 2002, 116, 878-890.	3.0	100
8	Second Quantized Approach to Quantum Chemistry. , 1989, , .		94
9	NDDO fragment self-consistent field approximation for large electronic systems. Journal of Computational Chemistry, 1992, 13, 830-837.	3.3	85
10	On the perturbation of multiconfiguration wave functions. Journal of Chemical Physics, 2003, 119, 1922-1928.	3.0	82
11	Electronic structure and optical absorption of poly(biisothianaphthene-methine) and poly(isonaphthothiophene-thiophene): two low-band-gap polymers. Journal of the American Chemical Society, 1991, 113, 9865-9867.	13.7	77
12	Improved intermolecularSCFtheory and theBSSEproblem. International Journal of Quantum Chemistry, 1989, 36, 225-240.	2.0	68
13	Strongly orthogonal geminals: size-extensive and variational reference states. Journal of Mathematical Chemistry, 2012, 50, 534-551.	1.5	68
14	Interruption of conjugations of polyacetylene chains. Physical Review B, 1986, 33, 2615-2624.	3.2	63
15	Comparison of low-order multireference many-body perturbation theories. Journal of Chemical Physics, 2005, 122, 134105.	3.0	62
16	Intershell interaction in double walled carbon nanotubes: Charge transfer and orbital mixing. Physical Review B, 2008, 77, .	3.2	61
17	Covalent bond orders and atomic valences from correlated wavefunctions. Chemical Physics Letters, 1999, 299, 1-8.	2.6	60
18	Localization and delocalization: Distinction between through space and through bond interactions. Journal of Chemical Physics, 1982, 77, 2454-2459.	3.0	55

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19	Scanning tunnelling microscopy (STM) imaging of carbon nanotubes. Carbon, 1998, 36, 689-696.	10.3	54
20	Multiconfiguration perturbation theory: Size consistency at second order. Journal of Chemical Physics, 2005, 122, 114104.	3.0	54
21	The MP2 energy as a functional of the Hartreeâ€“Fock density matrix. Chemical Physics Letters, 2005, 406, 318-320.	2.6	53
22	Generalized MÃ¸llerâ€'Plesset Partitioning in Multiconfiguration Perturbation Theory. Journal of Chemical Theory and Computation, 2010, 6, 2024-2033.	5.3	53
23	Comparative study of multireference perturbative theories for ground and excited states. Journal of Chemical Physics, 2009, 131, 204104.	3.0	51
24	Quinoid vs aromatic structure of polyisothianaphthene. Journal of Chemical Physics, 1990, 92, 3247-3248.	3.0	49
25	Partitioning in multiconfiguration perturbation theory. Annalen Der Physik, 2004, 13, 223-231.	2.4	45
26	Second-quantization-based perturbation theory for intermolecular interactions without basis set superposition error. Chemical Physics Letters, 1985, 119, 538-542.	2.6	43
27	Optimized partitioning in perturbation theory: Comparison to related approaches. Journal of Chemical Physics, 2000, 112, 4438-4446.	3.0	43
28	Bond orbital framework for rapid calculation of environmental effects on molecular potential surfaces. Chemical Physics Letters, 1983, 96, 499-501.	2.6	42
29	Interaction of chemical bonds. II.Ab initiotheory for overlap, delocalization, and dispersion interactions. Physical Review A, 1985, 32, 748-755.	2.5	42
30	Linearized Coupled Cluster Corrections to Antisymmetrized Product of Strongly Orthogonal Geminals: Role of Dispersive Interactions. Journal of Chemical Theory and Computation, 2013, 9, 2602-2608.	5.3	42
31	Intertube interactions in carbon nanotube bundles. Physical Review B, 2006, 73, .	3.2	41
32	Localization and delocalization. II. Role of overlap in interbond interactions. Journal of Chemical Physics, 1984, 80, 5649-5658.	3.0	40
33	Interaction of chemical bonds: Strictly localized wave functions in orthogonal basis. Physical Review A, 1984, 30, 43-50.	2.5	40
34	Perspectives of APSGâ€based multireference perturbation theories. International Journal of Quantum Chemistry, 2014, 114, 1048-1052.	2.0	39
35	Natural orbitals in CIS and singular-value decomposition. Chemical Physics Letters, 2007, 439, 393-394.	2.6	38
36	Intermolecular interactions using small basis sets: Perturbation theory calculations avoiding basis set superposition error. Chemical Physics Letters, 1986, 128, 358-362.	2.6	37

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37	Zero-field-splitting in the lowest triplet state of C60. Chemical Physics Letters, 1996, 251, 115-118.	2.6	37
38	Trapping of phase kinks in polyacetylene. Solid State Communications, 1981, 39, 611-614.	1.9	36
39	Design of small gap conjugated polymers. Synthetic Metals, 1993, 57, 4338-4343.	3.9	36
40	Perturbation theory for nonlinear time-independent SchrÃ¶dinger equations. Physical Review A, 1983, 28, 45-48.	2.5	35
41	Interaction of chemical bonds. V. Perturbative corrections to geminal-type wave functions. International Journal of Quantum Chemistry, 2000, 80, 96-104.	2.0	35
42	Band structures of neutral and doped (C60)x polymers. Solid State Communications, 1994, 92, 407-411.	1.9	34
43	Zeroâ€fieldâ€splitting and Ï€â€electron spin densities in the lowest excited triplet state of oligothiophenes. Journal of Chemical Physics, 1996, 105, 4441-4447.	3.0	34
44	Optimized partitioning in Rayleighâ€“SchrÃ¶dinger perturbation theory. Chemical Physics Letters, 1999, 308, 303-309.	2.6	34
45	Semiconductor-to-metal transition of double walled carbon nanotubes induced by inter-shell interaction. Physica Status Solidi (B): Basic Research, 2006, 243, 3476-3479.	1.5	30
46	Strictly localized molecular orbitals. Journal of the Chemical Society, Faraday Transactions 2, 1981, 77, 1129-1131.	1.1	28
47	Delocalization corrections to the strictly localized molecular orbitals: A linearized SCF approximation. Theoretica Chimica Acta, 1981, 59, 603-607.	0.8	28
48	Theoretical estimation of static charge fluctuation in amorphous silicon. Physical Review B, 1988, 37, 9069-9071.	3.2	27
49	Electronic excitations in fullerenes: Jahnâ€”Teller distorted structures of C60. Computational and Theoretical Chemistry, 1994, 311, 55-68.	1.5	27
50	The interaction of chemical bonds. III. Perturbed strictly localized geminals inLMObasis. International Journal of Quantum Chemistry, 1994, 52, 563-574.	2.0	26
51	Triplet State Characteristics of Higher Fullerenes. Journal of Physical Chemistry A, 1998, 102, 1261-1273.	2.5	26
52	Direct determination of fragment localized molecular orbitals and the orthogonality constraint. Chemical Physics Letters, 2003, 369, 125-130.	2.6	26
53	A sparse matrix based full-configuration interaction algorithm. Journal of Chemical Physics, 2008, 128, 144101.	3.0	26
54	Diagonalization-free initial guess to SCF calculations for large molecules. Chemical Physics Letters, 2006, 424, 420-424.	2.6	25

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55	Local spin from strongly orthogonal geminal wavefunctions. Molecular Physics, 2015, 113, 249-259.	1.7	23
56	Connected moments expansion calculations of the correlation energy in small molecules. Chemical Physics Letters, 1987, 138, 516-519.	2.6	22
57	The interaction of chemical bonds. IV. Interbond charge transfer by a coupled-cluster-type formalism. International Journal of Quantum Chemistry, 1995, 55, 109-116.	2.0	22
58	Electronic structure of the singly bonded(C60)xfullerene polymer. Physical Review B, 1998, 58, 3490-3493.	3.2	22
59	The reliability of the point charge model representing intermolecular effects in ab initio calculations. Chemical Physics Letters, 1994, 225, 258-264.	2.6	21
60	An effective hopping model for weakly interacting Ï€ systems: Electronic structure of stacked polyaromatic hydrocarbons. International Journal of Quantum Chemistry, 2001, 84, 216-225.	2.0	18
61	Intermolecular interactions: biorthogonal perturbation theory revisited. Computational and Theoretical Chemistry, 1991, 226, 47-58.	1.5	17
62	Electronic transition moments and optical absorption for trans-polyacetylene. Solid State Communications, 1983, 48, 243-247.	1.9	16
63	The application of strictly localized geminals to the description of chemical bonds. Journal of Computational Chemistry, 1987, 8, 436-441.	3.3	16
64	Energy, geometry and valence: The influence of sulfur d-orbital exponent. Computational and Theoretical Chemistry, 1988, 165, 297-307.	1.5	16
65	Damping of perturbation corrections in quasidegenerate situations. Journal of Chemical Physics, 1996, 104, 3320-3324.	3.0	16
66	Improving CISD calculations by geminal-type reference states. Chemical Physics Letters, 1999, 312, 221-228.	2.6	16
67	An ab initio study of the H2O-mediated 1,3-hydrogen rearrangement in the isoelectric series: X, Yâ€,=â€,CH2, NH, or O. Canadian Journal of Chemistry, 1991, 69, 1589-1599.	1.1	15
68	sp3 Hybridized carbons on buckminsterfullerene. Computational and Theoretical Chemistry, 1995, 338, 215-223.	1.5	15
69	On the â€œkiller conditionâ€™ in the equation-of-motion method: ionization potentials from multi-reference wave functions. Physical Chemistry Chemical Physics, 2001, 3, 696-701.	2.8	15
70	On the convergence of the coupled-cluster sequence: the H8 model. Computational and Theoretical Chemistry, 2001, 547, 145-151.	1.5	15
71	Spin Symmetry and Size Consistency of Strongly Orthogonal Geminals. Journal of Chemical Theory and Computation, 2015, 11, 3096-3103.	5.3	15
72	Ab initionumerical studies on density-matrix asymptotics in extended systems. Physical Review B, 1983, 27, 7583-7588.	3.2	14

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73	Quantum chemical conformational analysis of the catalytic triad in Î±-chymotrypsin. Computational and Theoretical Chemistry, 1985, 123, 85-95.	1.5	14
74	Effect of protonation on the ground state properties of retinal analogs: an ab-initio study. Canadian Journal of Chemistry, 1987, 65, 892-897.	1.1	14
75	Orthogonality constrained excited states. Chemical Physics Letters, 2000, 325, 120-126.	2.6	14
76	Nonsymmetrical perturbation theory for improving coupled-cluster wave functions. International Journal of Quantum Chemistry, 2002, 90, 1309-1320.	2.0	14
77	Idempotency-Conserving Iteration Scheme for the One-Electron Density Matrix. Physical Review Letters, 2005, 95, 013002.	7.8	14
78	Spin-adaptation and redundancy in state-specific multireference perturbation theory. Journal of Chemical Physics, 2013, 138, 124110.	3.0	14
79	Half-Projection of the Strongly Orthogonal Unrestricted Geminalsâ€™ Product Wave Function. Journal of Chemical Theory and Computation, 2020, 16, 892-903.	5.3	14
80	Conformational analysis by bond orbitals with delocalization corrections: Rotation of the ser-195 side chain in Î±-chymotrypsin. International Journal of Quantum Chemistry, 1982, 22, 929-938.	2.0	13
81	Normalization corrections to perturbation theory for the time-independent nonlinear SchrÃ¶dinger equation. Physical Review A, 1991, 44, 2188-2191.	2.5	13
82	Laplace-transformed denominators in perturbation theory: Linear-scaling second-order treatment of weakly interacting nanostructures. Physical Review A, 2003, 68, .	2.5	13
83	Stability conditions for the coupled cluster equations. International Journal of Quantum Chemistry, 2008, 108, 2043-2052.	2.0	13
84	Role of triplet states in geminal-based perturbation theory. Molecular Physics, 2015, 113, 2960-2963.	1.7	13
85	Quinoid-Aromatic Transition in Polythiophene-like Systems. Springer Series in Solid-state Sciences, 1989, , 69-72.	0.3	13
86	Appendix to â€œStudies in Perturbation Theoryâ€: The Problem of Partitioning. , 2004, , 129-185.		13
87	Nitrogen bridgehead compounds. 48. Synthesis and stereochemistry of 4-oxo-1,6,7,8,9,9a-hexahydro-4H-pyrido[1,2-a]pyrimidine-3-carboxamides. Journal of Organic Chemistry, 1985, 50, 2918-2925.	3.2	12
88	Third-order many-body perturbation theory for intermolecular interactions. I. Hartree-Fock level. , 1997, 64, 43-51.		12
89	Nonconventional partitioning of the many-body Hamiltonian for studying correlation effects. International Journal of Quantum Chemistry, 1998, 70, 571-581.	2.0	12
90	Theoretical CD spectrum calculations of the crown-ether aralkyl-ammonium salt complex. Chirality, 2002, 14, 377-385.	2.6	12

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91	Constant denominator perturbative schemes and the partitioning technique. International Journal of Quantum Chemistry, 2002, 90, 20-26.	2.0	12
92	Mayerâ€™s orthogonalization: relation to the Gram-Schmidt and LÃ¶wdinâ€™s symmetrical scheme. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	12
93	Circular dichroism of host-guest complexes of achiral pyridino- and phenazino-18-crown-6 ligands with the enantiomers of chiral aralkyl ammonium salts. Chirality, 2001, 13, 109-117.	2.6	11
94	Stability and Properties of Polyhelicenes and Annelated Fused-Ring Carbon Helices:Â Models Toward Helical Graphites. Journal of Chemical Information and Modeling, 2005, 45, 850-855.	5.4	11
95	Iterative solution of Bloch-type equations: stability conditions and chaotic behavior. Journal of Mathematical Chemistry, 2008, 43, 314-327.	1.5	11
96	Bondâ€”bond pair potentials describing barrier to rotations around single bonds. Chemical Physics Letters, 1982, 92, 483-485.	2.6	10
97	Nitrogen bridgehead compounds. Part 32. Absolute configuration and circular dichroism of 6-methyl-tetrahydro-4H-pyrido[1,2-a]pyrimidin-4-ones. Journal of the Chemical Society Perkin Transactions II, 1983, , 1413-1420.	0.9	10
98	Electronic excitations in fullerenes: Jahn-Teller distorted structures of C60. Journal of Molecular Structure, 1994, 311, 55-68.	3.6	10
99	Analytic-continuation approach to the resummation of divergent series in Rayleigh-SchrÃ¶dinger perturbation theory. Physical Review A, 2017, 96, .	2.5	10
100	Geminal perturbation theory based on the unrestricted Hartreeâ€“Fock wavefunction. Journal of Chemical Physics, 2019, 150, 034103.	3.0	10
101	A preliminary ab initio investigation of retinal analogs. Computational and Theoretical Chemistry, 1988, 167, 321-329.	1.5	9
102	Ab initio Hartree- Fock calculations of the interaction energy of bimolecular complexes. Computational and Theoretical Chemistry, 1994, 307, 239-259.	1.5	9
103	Excited states of the C60 dimer. Synthetic Metals, 1996, 77, 107-110.	3.9	9
104	Dyson-corrected orbital energies for the perturbative treatment of electron correlation. International Journal of Quantum Chemistry, 1998, 69, 713-719.	2.0	9
105	On the Use of Connected Moments Expansion with Coupled Cluster Reference. International Journal of Molecular Sciences, 2002, 3, 508-521.	4.1	9
106	Jahnâ€“Teller distortion of ionized and excited carbon nanotubes. Journal of Chemical Physics, 2010, 132, 034309.	3.0	9
107	Resonance Raman Optical Activity of Single Walled Chiral Carbon Nanotubes. Journal of Physical Chemistry A, 2016, 120, 5527-5538.	2.5	9
108	Convergence Enhancement in Perturbation Theory. Collection of Czechoslovak Chemical Communications, 2004, 69, 105-120.	1.0	8

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109	Application of the Cauchy integral formula as a tool of analytic continuation for the resummation of divergent perturbation series. Journal of Chemical Physics, 2019, 150, 031101.	3.0	8
110	Bond orbital approach for optical rotatory strength calculations. Theoretica Chimica Acta, 1983, 63, 43-54.	0.8	7
111	Embedded units in conjugated polymers. Journal of Mathematical Chemistry, 1992, 10, 313-327.	1.5	7
112	Energetics and zero-field-splitting in triplet states of C70. Computational and Theoretical Chemistry, 1997, 398-399, 293-300.	1.5	7
113	The phase diagram of charge- and spin-density waves in polymeric C 60. Applied Physics A: Materials Science and Processing, 1997, 64, 315-319.	2.3	7
114	Optimized Quasiparticle Energies in Many-Body Perturbation Theory. Collection of Czechoslovak Chemical Communications, 2003, 68, 331-339.	1.0	7
115	Second quantization and the Hellmannâ€"Feynman Theorem: A unified view on energy derivatives. Computational and Theoretical Chemistry, 1988, 170, 1-7.	1.5	6
116	Perturbation theoretical vs supermolecule calculations on intermolecular interactions. Acta Physica Hungarica, 1990, 67, 387-400.	0.1	6
117	Size dependence of Feenberg scaling. International Journal of Quantum Chemistry, 2005, 101, 287-290.	2.0	6
118	Coupled-cluster theory and the method of moments. Computational and Theoretical Chemistry, 2006, 768, 17-23.	1.5	6
119	Frozen localized molecular orbitals in electron correlation calculations â€“ Exploiting the Hartreeâ€"Fock density matrix. Chemical Physics Letters, 2008, 450, 400-403.	2.6	6
120	Efficient iterative diagonalization of the Boseâ€"Hubbard model for ultracold bosons in a periodic optical trap. Chemical Physics, 2012, 401, 208-216.	1.9	6
121	Theoretical vibrational optical activity of chiral carbon nanoparticles: Fullerenes and carbon nanotubes. Physica Status Solidi (B): Basic Research, 2014, 251, 2451-2456.	1.5	6
122	Effect of partitioning on the convergence properties of the Rayleigh-SchrÃ¶dinger perturbation series. Journal of Chemical Physics, 2017, 146, 124121.	3.0	6
123	The inverse boundary value problem: application in many-body perturbation theory. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	6
124	Jahn-Teller Distorted Excited States of C60. Springer Series in Solid-state Sciences, 1993, , 126-130.	0.3	6
125	On the perturbation operator in ab initio theories of intermolecular interactions. Computational and Theoretical Chemistry, 1991, 226, 39-46.	1.5	5
126	Optical spectra of diels-alder adducts of C60. Synthetic Metals, 1995, 70, 1377-1378.	3.9	5

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127	Charge vs. spin density waves in the fullerene polymer. , 1997, 63, 425-435.		5
128	Near-degeneracy corrections for second-order perturbation theory: comparison of two approaches. Theoretical Chemistry Accounts, 2001, 105, 408-412.	1.4	5
129	Vibrational optical activity of chiral carbon nanoclusters treated by a generalized Ï€-electron method. Journal of Chemical Physics, 2014, 140, 044112.	3.0	5
130	Improving half-projected spin-contaminated wave functions by multi-configuration perturbation theory. Journal of Chemical Physics, 2021, 154, 234110.	3.0	5
131	The use of the mulliken approximation in bond-bond pair potentials describing rotational barriers. Chemical Physics Letters, 1985, 117, 386-388.	2.6	4
132	Second quantization and exchange perturbation theory for intermolecular interactions. the basis set superposition error problem. Computational and Theoretical Chemistry, 1991, 232, 51-63.	1.5	4
133	Nonlinear schrï¿½dinger equations and intermolecular interactions. Journal of Mathematical Chemistry, 1991, 8, 151-160.	1.5	4
134	Searching for low-band-gap conjugated polymers by LHS calculations. Synthetic Metals, 1992, 50, 537-542.	3.9	4
135	Localization maps by orbital partitioning of the electron density. Theoretica Chimica Acta, 1993, 86, 379-389.	0.8	4
136	Perturbative calculation of intermolecular interactions in orthogonalized or biorthogonal basis sets. Theoretica Chimica Acta, 1996, 94, 333-344.	0.8	4
137	Calculation of correlation-corrected band structures of polymers in the case of quasi-degeneracy. Solid State Communications, 1997, 103, 639-644.	1.9	4
138	Optimized partitioning in PT: Application for the equation of motion describing ionization processes. International Journal of Quantum Chemistry, 2003, 92, 160-167.	2.0	4
139	Zero-field-splitting in triplet-state nanotubes. Chemical Physics Letters, 2010, 498, 292-295.	2.6	4
140	Introducing the Î³ function in quantum theory. International Journal of Quantum Chemistry, 2020, 120, e26221.	2.0	4
141	Symmetry-Adapted Perturbation with Half-Projection for Spin Unrestricted Geminals. Journal of Chemical Theory and Computation, 2021, 17, 4122-4143.	5.3	4
142	The Two-Electron Bond as a Molecular Building Block. , 1990, , 205-256.		4
143	Fermi-Vacuum Invariance in Multiconfiguration Perturbation Theory. Progress in Theoretical Chemistry and Physics, 2009, , 257-268.	0.2	4
144	Optical rotatory strength calculation by evaluating the gradient matrix through the equation of motion. Theoretica Chimica Acta, 1980, 55, 103-115.	0.8	3

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145	The role of hybridization in perturbative bond theories: The existence of exact strictly localized orbitals in small molecules. Computational and Theoretical Chemistry, 1988, 169, 95-104.	1.5	3
146	Computational chemistry on a PC. International Journal of Quantum Chemistry, 1990, 38, 163-171.	2.0	3
147	Quinoid-aromatic competition as a tool for band structure design for conjugated polymers. Synthetic Metals, 1993, 57, 4260-4265.	3.9	3
148	Distorted s-type orbitals: the $${m H}^{+}_{2}$$ problem revisited. Journal of Mathematical Chemistry, 2008, 43, 227-236.	1.5	3
149	Effectiveï€-electron Hamiltonian for small-radius nanotubes: Interpretation of curvature-induced conductivity. Physical Review B, 2008, 77, .	3.2	3
150	On Trapping of Phase Kinks in Polyacetylene. Molecular Crystals and Liquid Crystals, 1981, 77, 341-348.	0.8	2
151	Impurity-induced tetramerization in Peierls-distorted polymers: Reducing the band gap. Solid State Communications, 1991, 77, 875-877.	1.9	2
152	Interaction energies between H2O and HXâ€”CH=Y/X=CHâ€”YH for X, Y=CH2, NH or O â€” the chemical Hamiltonian approach. Chemical Physics Letters, 1991, 183, 25-30.	2.6	2
153	Triplet State Characteristics of Smaller Fullerenes. Fullerenes, Nanotubes, and Carbon Nanostructures, 1997, 5, 355-373.	0.6	2
154	A stationary property of the APSG wave function. Journal of Mathematical Chemistry, 2011, 49, 1217-1225.	1.5	2
155	A Note on the Symmetry Properties of LÃ¶wdin's Orthogonalization Schemes. Collection of Czechoslovak Chemical Communications, 2008, 73, 937-944.	1.0	2
156	Hybridization effects in localized wave functions. Computational and Theoretical Chemistry, 1998, 455, 175-182.	1.5	1
157	The nature of electronic excitations in singly bonded C 60 dimer. Computational and Theoretical Chemistry, 2000, 501-502, 369-377.	1.5	1
158	Composite particles in quantum chemistry: From twoâ€electron bonds to cold atoms. International Journal of Quantum Chemistry, 2013, 113, 185-189.	2.0	1
159	Perturbative Approximations to Avoid Matrix Diagonalization. Challenges and Advances in Computational Chemistry and Physics, 2011, , 83-95.	0.6	1
160	On The Coupled-Cluster Equations. Stability Analysis And Nonstandard Correction Schemes. Challenges and Advances in Computational Chemistry and Physics, 2010, , 513-534.	0.6	1
161	Stability analysis of the Lippmannâ€“Schwinger equation. Molecular Physics, 2023, 121, .	1.7	1
162	Highly symmetric borane clusters as fullerene analogs. , 1998, , .		0

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163	Stability and Properties of Polyhelicenes and Anellated Fused-Ring Carbon Helices: Models Toward Helical Graphites.. ChemInform, 2005, 36, no.	0.0	0
164	The high-rank Hartreeâ€“Fock method as an averaging procedure. Molecular Physics, 2006, 104, 2037-2046.	1.7	0
165	BSSE-free SCF methods for intermolecular interactions. International Journal of Quantum Chemistry, 1989, 36, 281-290.	2.0	0
166	Editorial: in memoriam JÃ¡nos G. Ã•gyÃ¡n (1956â€“2017). Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	0
167	On the variational principle for the non-linear SchrÃ¶dinger equation. Journal of Mathematical Chemistry, 2020, 58, 340-351.	1.5	0
168	Comment on â€œImproved many-body expansions from eigenvector continuationâ€• Physical Review C, 2021, 103, .	2.9	0
169	The $$gamma$$ function in quantum theory II. Mathematical challenges and paradoxa. Journal of Mathematical Chemistry, 2022, 60, 267-282.	1.5	0
170	Editorial: In memoriam IstvÃ¡n Mayer. International Journal of Quantum Chemistry, 2022, 122, .	2.0	0
171	A note on perturbation-adapted perturbation theory. Journal of Chemical Physics, 2022, 156, 116102.	3.0	0
172	Many-Body Perturbation Theory with Localized Orbitals: Accounting for Localization Diagrams as Integral Dressing. Journal of Chemical Theory and Computation, 2022, , .	5.3	0
173	Quantum chemical conformational analysis of the catalytic triad in Î±-chymotrypsin. Computational and Theoretical Chemistry, 1985, 24, 85-95.	1.5	0