

Peter R Surján

List of Publications by Year in descending order

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173
papers

4,579
citations

109137

35
h-index

128067

60
g-index

183
all docs

183
docs citations

183
times ranked

2218
citing authors

#	ARTICLE	IF	CITATIONS
1	Higher excitations in coupled-cluster theory. <i>Journal of Chemical Physics</i> , 2001, 115, 2945-2954.	1.2	666
2	A general state-selective multireference coupled-cluster algorithm. <i>Journal of Chemical Physics</i> , 2002, 117, 980-990.	1.2	237
3	An observable-based interpretation of electronic wavefunctions: application to hypervalent molecules. <i>Computational and Theoretical Chemistry</i> , 1992, 255, 9-33.	1.5	137
4	Computing coupled-cluster wave functions with arbitrary excitations. <i>Journal of Chemical Physics</i> , 2000, 113, 1359-1365.	1.2	127
5	An Introduction to the Theory of Geminals. <i>Topics in Current Chemistry</i> , 1999, , 63-88.	4.0	115
6	Monomer geometry relaxation and the basis set superposition error. <i>Chemical Physics Letters</i> , 1992, 191, 497-499.	1.2	113
7	Two-body zeroth order Hamiltonians in multireference perturbation theory: The APSG reference state. <i>Journal of Chemical Physics</i> , 2002, 116, 878-890.	1.2	100
8	Second Quantized Approach to Quantum Chemistry. , 1989, , .		94
9	NDDO fragment self-consistent field approximation for large electronic systems. <i>Journal of Computational Chemistry</i> , 1992, 13, 830-837.	1.5	85
10	On the perturbation of multiconfiguration wave functions. <i>Journal of Chemical Physics</i> , 2003, 119, 1922-1928.	1.2	82
11	Electronic structure and optical absorption of poly(bisothianaphthene-methine) and poly(isonaphthothiophene-thiophene): two low-band-gap polymers. <i>Journal of the American Chemical Society</i> , 1991, 113, 9865-9867.	6.6	77
12	Improved intermolecular SCF theory and the BSSE problem. <i>International Journal of Quantum Chemistry</i> , 1989, 36, 225-240.	1.0	68
13	Strongly orthogonal geminals: size-extensive and variational reference states. <i>Journal of Mathematical Chemistry</i> , 2012, 50, 534-551.	0.7	68
14	Interruption of conjugations of polyacetylene chains. <i>Physical Review B</i> , 1986, 33, 2615-2624.	1.1	63
15	Comparison of low-order multireference many-body perturbation theories. <i>Journal of Chemical Physics</i> , 2005, 122, 134105.	1.2	62
16	Intershell interaction in double walled carbon nanotubes: Charge transfer and orbital mixing. <i>Physical Review B</i> , 2008, 77, .	1.1	61
17	Covalent bond orders and atomic valences from correlated wavefunctions. <i>Chemical Physics Letters</i> , 1999, 299, 1-8.	1.2	60
18	Localization and delocalization: Distinction between through space and through bond interactions. <i>Journal of Chemical Physics</i> , 1982, 77, 2454-2459.	1.2	55

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19	Scanning tunnelling microscopy (STM) imaging of carbon nanotubes. <i>Carbon</i> , 1998, 36, 689-696.	5.4	54
20	Multiconfiguration perturbation theory: Size consistency at second order. <i>Journal of Chemical Physics</i> , 2005, 122, 114104.	1.2	54
21	The MP2 energy as a functional of the Hartree-Fock density matrix. <i>Chemical Physics Letters</i> , 2005, 406, 318-320.	1.2	53
22	Generalized Møller-Plesset Partitioning in Multiconfiguration Perturbation Theory. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2024-2033.	2.3	53
23	Comparative study of multireference perturbative theories for ground and excited states. <i>Journal of Chemical Physics</i> , 2009, 131, 204104.	1.2	51
24	Quinoid vs aromatic structure of polyisothianaphthene. <i>Journal of Chemical Physics</i> , 1990, 92, 3247-3248.	1.2	49
25	Partitioning in multiconfiguration perturbation theory. <i>Annalen Der Physik</i> , 2004, 13, 223-231.	0.9	45
26	Second-quantization-based perturbation theory for intermolecular interactions without basis set superposition error. <i>Chemical Physics Letters</i> , 1985, 119, 538-542.	1.2	43
27	Optimized partitioning in perturbation theory: Comparison to related approaches. <i>Journal of Chemical Physics</i> , 2000, 112, 4438-4446.	1.2	43
28	Bond orbital framework for rapid calculation of environmental effects on molecular potential surfaces. <i>Chemical Physics Letters</i> , 1983, 96, 499-501.	1.2	42
29	Interaction of chemical bonds. II. Ab initio theory for overlap, delocalization, and dispersion interactions. <i>Physical Review A</i> , 1985, 32, 748-755.	1.0	42
30	Linearized Coupled Cluster Corrections to Antisymmetrized Product of Strongly Orthogonal Geminals: Role of Dispersive Interactions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2602-2608.	2.3	42
31	Intertube interactions in carbon nanotube bundles. <i>Physical Review B</i> , 2006, 73, .	1.1	41
32	Localization and delocalization. II. Role of overlap in interbond interactions. <i>Journal of Chemical Physics</i> , 1984, 80, 5649-5658.	1.2	40
33	Interaction of chemical bonds: Strictly localized wave functions in orthogonal basis. <i>Physical Review A</i> , 1984, 30, 43-50.	1.0	40
34	Perspectives of APSC-based multireference perturbation theories. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 1048-1052.	1.0	39
35	Natural orbitals in CIS and singular-value decomposition. <i>Chemical Physics Letters</i> , 2007, 439, 393-394.	1.2	38
36	Intermolecular interactions using small basis sets: Perturbation theory calculations avoiding basis set superposition error. <i>Chemical Physics Letters</i> , 1986, 128, 358-362.	1.2	37

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37	Zero-field-splitting in the lowest triplet state of C60. <i>Chemical Physics Letters</i> , 1996, 251, 115-118.	1.2	37
38	Trapping of phase kinks in polyacetylene. <i>Solid State Communications</i> , 1981, 39, 611-614.	0.9	36
39	Design of small gap conjugated polymers. <i>Synthetic Metals</i> , 1993, 57, 4338-4343.	2.1	36
40	Perturbation theory for nonlinear time-independent Schrödinger equations. <i>Physical Review A</i> , 1983, 28, 45-48.	1.0	35
41	Interaction of chemical bonds. V. Perturbative corrections to geminal-type wave functions. <i>International Journal of Quantum Chemistry</i> , 2000, 80, 96-104.	1.0	35
42	Band structures of neutral and doped (C60) _x polymers. <i>Solid State Communications</i> , 1994, 92, 407-411.	0.9	34
43	Zero-field-splitting and electron spin densities in the lowest excited triplet state of oligothiophenes. <i>Journal of Chemical Physics</i> , 1996, 105, 4441-4447.	1.2	34
44	Optimized partitioning in Rayleigh-Schrödinger perturbation theory. <i>Chemical Physics Letters</i> , 1999, 308, 303-309.	1.2	34
45	Semiconductor-to-metal transition of double walled carbon nanotubes induced by inter-shell interaction. <i>Physica Status Solidi (B): Basic Research</i> , 2006, 243, 3476-3479.	0.7	30
46	Strictly localized molecular orbitals. <i>Journal of the Chemical Society, Faraday Transactions 2</i> , 1981, 77, 1129-1131.	1.1	28
47	Delocalization corrections to the strictly localized molecular orbitals: A linearized SCF approximation. <i>Theoretica Chimica Acta</i> , 1981, 59, 603-607.	0.9	28
48	Theoretical estimation of static charge fluctuation in amorphous silicon. <i>Physical Review B</i> , 1988, 37, 9069-9071.	1.1	27
49	Electronic excitations in fullerenes: Jahn-Teller distorted structures of C60. <i>Computational and Theoretical Chemistry</i> , 1994, 311, 55-68.	1.5	27
50	The interaction of chemical bonds. III. Perturbed strictly localized geminals in LMO basis. <i>International Journal of Quantum Chemistry</i> , 1994, 52, 563-574.	1.0	26
51	Triplet State Characteristics of Higher Fullerenes. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1261-1273.	1.1	26
52	Direct determination of fragment localized molecular orbitals and the orthogonality constraint. <i>Chemical Physics Letters</i> , 2003, 369, 125-130.	1.2	26
53	A sparse matrix based full-configuration interaction algorithm. <i>Journal of Chemical Physics</i> , 2008, 128, 144101.	1.2	26
54	Diagonalization-free initial guess to SCF calculations for large molecules. <i>Chemical Physics Letters</i> , 2006, 424, 420-424.	1.2	25

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55	Local spin from strongly orthogonal geminal wavefunctions. <i>Molecular Physics</i> , 2015, 113, 249-259.	0.8	23
56	Connected moments expansion calculations of the correlation energy in small molecules. <i>Chemical Physics Letters</i> , 1987, 138, 516-519.	1.2	22
57	The interaction of chemical bonds. IV. Interbond charge transfer by a coupled-cluster-type formalism. <i>International Journal of Quantum Chemistry</i> , 1995, 55, 109-116.	1.0	22
58	Electronic structure of the singly bonded(C60)xfullerene polymer. <i>Physical Review B</i> , 1998, 58, 3490-3493.	1.1	22
59	The reliability of the point charge model representing intermolecular effects in ab initio calculations. <i>Chemical Physics Letters</i> , 1994, 225, 258-264.	1.2	21
60	An effective hopping model for weakly interacting π systems: Electronic structure of stacked polyaromatic hydrocarbons. <i>International Journal of Quantum Chemistry</i> , 2001, 84, 216-225.	1.0	18
61	Intermolecular interactions: biorthogonal perturbation theory revisited. <i>Computational and Theoretical Chemistry</i> , 1991, 226, 47-58.	1.5	17
62	Electronic transition moments and optical absorption for trans-polyacetylene. <i>Solid State Communications</i> , 1983, 48, 243-247.	0.9	16
63	The application of strictly localized geminals to the description of chemical bonds. <i>Journal of Computational Chemistry</i> , 1987, 8, 436-441.	1.5	16
64	Energy, geometry and valence: The influence of sulfur d-orbital exponent. <i>Computational and Theoretical Chemistry</i> , 1988, 165, 297-307.	1.5	16
65	Damping of perturbation corrections in quasidegenerate situations. <i>Journal of Chemical Physics</i> , 1996, 104, 3320-3324.	1.2	16
66	Improving CISD calculations by geminal-type reference states. <i>Chemical Physics Letters</i> , 1999, 312, 221-228.	1.2	16
67	An ab initio study of the H ₂ O-mediated 1,3-hydrogen rearrangement in the isoelectric series: X, Y = C, CH ₂ , NH, or O. <i>Canadian Journal of Chemistry</i> , 1991, 69, 1589-1599.	0.6	15
68	sp ³ Hybridized carbons on buckminsterfullerene. <i>Computational and Theoretical Chemistry</i> , 1995, 338, 215-223.	1.5	15
69	On the "killer condition" in the equation-of-motion method: ionization potentials from multi-reference wave functions. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 696-701.	1.3	15
70	On the convergence of the coupled-cluster sequence: the H8 model. <i>Computational and Theoretical Chemistry</i> , 2001, 547, 145-151.	1.5	15
71	Spin Symmetry and Size Consistency of Strongly Orthogonal Geminals. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3096-3103.	2.3	15
72	Ab initio numerical studies on density-matrix asymptotics in extended systems. <i>Physical Review B</i> , 1983, 27, 7583-7588.	1.1	14

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73	Quantum chemical conformational analysis of the catalytic triad in β -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 <i>ab initio</i> study. Canadian Journal of Chemistry, 1987, 65, 892-897.	0.6	14
75	Orthogonality constrained excited states. Chemical Physics Letters, 2000, 325, 120-126.	1.2	14
76	Nonsymmetrical perturbation theory for improving coupled-cluster wave functions. International Journal of Quantum Chemistry, 2002, 90, 1309-1320.	1.0	14
77	Idempotency-Conserving Iteration Scheme for the One-Electron Density Matrix. Physical Review Letters, 2005, 95, 013002.	2.9	14
78	Spin-adaptation and redundancy in state-specific multireference perturbation theory. Journal of Chemical Physics, 2013, 138, 124110.	1.2	14
79	Half-Projection of the Strongly Orthogonal Unrestricted Geminals TM Product Wave Function. Journal of Chemical Theory and Computation, 2020, 16, 892-903.	2.3	14
80	Conformational analysis by bond orbitals with delocalization corrections: Rotation of the ser-195 side chain in β -chymotrypsin. International Journal of Quantum Chemistry, 1982, 22, 929-938.	1.0	13
81	Normalization corrections to perturbation theory for the time-independent nonlinear Schrödinger equation. Physical Review A, 1991, 44, 2188-2191.	1.0	13
82	Laplace-transformed denominators in perturbation theory: Linear-scaling second-order treatment of weakly interacting nanostructures. Physical Review A, 2003, 68, .	1.0	13
83	Stability conditions for the coupled cluster equations. International Journal of Quantum Chemistry, 2008, 108, 2043-2052.	1.0	13
84	Role of triplet states in geminal-based perturbation theory. Molecular Physics, 2015, 113, 2960-2963.	0.8	13
85	Quinoid-Aromatic Transition in Polythiophene-like Systems. Springer Series in Solid-state Sciences, 1989, , 69-72.	0.3	13
86	Appendix to "Studies in Perturbation Theory": 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.	1.7	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.	1.0	12
90	Theoretical CD spectrum calculations of the crown-ether aralkyl-ammonium salt complex. Chirality, 2002, 14, 377-385.	1.3	12

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91	Constant denominator perturbative schemes and the partitioning technique. <i>International Journal of Quantum Chemistry</i> , 2002, 90, 20-26.	1.0	12
92	Mayer's orthogonalization: relation to the Gram-Schmidt and Löwdin's symmetrical scheme. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	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. <i>Chirality</i> , 2001, 13, 109-117.	1.3	11
94	Stability and Properties of Polyhelicenes and Annelated Fused-Ring Carbon Helices: Models Toward Helical Graphites. <i>Journal of Chemical Information and Modeling</i> , 2005, 45, 850-855.	2.5	11
95	Iterative solution of Bloch-type equations: stability conditions and chaotic behavior. <i>Journal of Mathematical Chemistry</i> , 2008, 43, 314-327.	0.7	11
96	Bond's bond pair potentials describing barrier to rotations around single bonds. <i>Chemical Physics Letters</i> , 1982, 92, 483-485.	1.2	10
97	Nitrogen bridgehead compounds. Part 32. Absolute configuration and circular dichroism of 6-methyl-tetrahydro-4H-pyrido[1,2-a]pyrimidin-4-ones. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1983, , 1413-1420.	0.9	10
98	Electronic excitations in fullerenes: Jahn-Teller distorted structures of C60. <i>Journal of Molecular Structure</i> , 1994, 311, 55-68.	1.8	10
99	Analytic-continuation approach to the resummation of divergent series in Rayleigh-Schrödinger perturbation theory. <i>Physical Review A</i> , 2017, 96, .	1.0	10
100	Geminal perturbation theory based on the unrestricted Hartree-Fock wavefunction. <i>Journal of Chemical Physics</i> , 2019, 150, 034103.	1.2	10
101	A preliminary ab initio investigation of retinal analogs. <i>Computational and Theoretical Chemistry</i> , 1988, 167, 321-329.	1.5	9
102	Ab initio Hartree- Fock calculations of the interaction energy of bimolecular complexes. <i>Computational and Theoretical Chemistry</i> , 1994, 307, 239-259.	1.5	9
103	Excited states of the C60 dimer. <i>Synthetic Metals</i> , 1996, 77, 107-110.	2.1	9
104	Dyson-corrected orbital energies for the perturbative treatment of electron correlation. <i>International Journal of Quantum Chemistry</i> , 1998, 69, 713-719.	1.0	9
105	On the Use of Connected Moments Expansion with Coupled Cluster Reference. <i>International Journal of Molecular Sciences</i> , 2002, 3, 508-521.	1.8	9
106	Jahn-Teller distortion of ionized and excited carbon nanotubes. <i>Journal of Chemical Physics</i> , 2010, 132, 034309.	1.2	9
107	Resonance Raman Optical Activity of Single Walled Chiral Carbon Nanotubes. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5527-5538.	1.1	9
108	Convergence Enhancement in Perturbation Theory. <i>Collection of Czechoslovak Chemical Communications</i> , 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. <i>Journal of Chemical Physics</i> , 2019, 150, 031101.	1.2	8
110	Bond orbital approach for optical rotatory strength calculations. <i>Theoretica Chimica Acta</i> , 1983, 63, 43-54.	0.9	7
111	Embedded units in conjugated polymers. <i>Journal of Mathematical Chemistry</i> , 1992, 10, 313-327.	0.7	7
112	Energetics and zero-field-splitting in triplet states of C70. <i>Computational and Theoretical Chemistry</i> , 1997, 398-399, 293-300.	1.5	7
113	The phase diagram of charge- and spin-density waves in polymeric C 60. <i>Applied Physics A: Materials Science and Processing</i> , 1997, 64, 315-319.	1.1	7
114	Optimized Quasiparticle Energies in Many-Body Perturbation Theory. <i>Collection of Czechoslovak Chemical Communications</i> , 2003, 68, 331-339.	1.0	7
115	Second quantization and the Hellmann-Feynman Theorem: A unified view on energy derivatives. <i>Computational and Theoretical Chemistry</i> , 1988, 170, 1-7.	1.5	6
116	Perturbation theoretical vs supermolecule calculations on intermolecular interactions. <i>Acta Physica Hungarica</i> , 1990, 67, 387-400.	0.1	6
117	Size dependence of Feenberg scaling. <i>International Journal of Quantum Chemistry</i> , 2005, 101, 287-290.	1.0	6
118	Coupled-cluster theory and the method of moments. <i>Computational and Theoretical Chemistry</i> , 2006, 768, 17-23.	1.5	6
119	Frozen localized molecular orbitals in electron correlation calculations – Exploiting the Hartree-Fock density matrix. <i>Chemical Physics Letters</i> , 2008, 450, 400-403.	1.2	6
120	Efficient iterative diagonalization of the Bose-Hubbard model for ultracold bosons in a periodic optical trap. <i>Chemical Physics</i> , 2012, 401, 208-216.	0.9	6
121	Theoretical vibrational optical activity of chiral carbon nanoparticles: Fullerenes and carbon nanotubes. <i>Physica Status Solidi (B): Basic Research</i> , 2014, 251, 2451-2456.	0.7	6
122	Effect of partitioning on the convergence properties of the Rayleigh-Schrödinger perturbation series. <i>Journal of Chemical Physics</i> , 2017, 146, 124121.	1.2	6
123	The inverse boundary value problem: application in many-body perturbation theory. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	6
124	Jahn-Teller Distorted Excited States of C60. <i>Springer Series in Solid-state Sciences</i> , 1993, , 126-130.	0.3	6
125	On the perturbation operator in ab initio theories of intermolecular interactions. <i>Computational and Theoretical Chemistry</i> , 1991, 226, 39-46.	1.5	5
126	Optical spectra of diels-alder adducts of C60. <i>Synthetic Metals</i> , 1995, 70, 1377-1378.	2.1	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.	0.5	5
129	Vibrational optical activity of chiral carbon nanoclusters treated by a generalized π -electron method. Journal of Chemical Physics, 2014, 140, 044112.	1.2	5
130	Improving half-projected spin-contaminated wave functions by multi-configuration perturbation theory. Journal of Chemical Physics, 2021, 154, 234110.	1.2	5
131	The use of the mulliken approximation in bond-bond pair potentials describing rotational barriers. Chemical Physics Letters, 1985, 117, 386-388.	1.2	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 schrödinger equations and intermolecular interactions. Journal of Mathematical Chemistry, 1991, 8, 151-160.	0.7	4
134	Searching for low-band-gap conjugated polymers by LHS calculations. Synthetic Metals, 1992, 50, 537-542.	2.1	4
135	Localization maps by orbital partitioning of the electron density. Theoretica Chimica Acta, 1993, 86, 379-389.	0.9	4
136	Perturbative calculation of intermolecular interactions in orthogonalized or biorthogonal basis sets. Theoretica Chimica Acta, 1996, 94, 333-344.	0.9	4
137	Calculation of correlation-corrected band structures of polymers in the case of quasi-degeneracy. Solid State Communications, 1997, 103, 639-644.	0.9	4
138	Optimized partitioning in PT: Application for the equation of motion describing ionization processes. International Journal of Quantum Chemistry, 2003, 92, 160-167.	1.0	4
139	Zero-field-splitting in triplet-state nanotubes. Chemical Physics Letters, 2010, 498, 292-295.	1.2	4
140	Introducing the $\langle i \hat{p}^3 i \rangle$ function in quantum theory. International Journal of Quantum Chemistry, 2020, 120, e26221.	1.0	4
141	Symmetry-Adapted Perturbation with Half-Projection for Spin Unrestricted Geminals. Journal of Chemical Theory and Computation, 2021, 17, 4122-4143.	2.3	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.	0.9	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.	1.0	3
147	Quinoid-aromatic competition as a tool for band structure design for conjugated polymers. Synthetic Metals, 1993, 57, 4260-4265.	2.1	3
148	Distorted s-type orbitals: the $\{m H^+\}_2$ problem revisited. Journal of Mathematical Chemistry, 2008, 43, 227-236.	0.7	3
149	Effective π -electron Hamiltonian for small-radius nanotubes: Interpretation of curvature-induced conductivity. Physical Review B, 2008, 77, .	1.1	3
150	On Trapping of Phase Kinks in Polyacetylene. Molecular Crystals and Liquid Crystals, 1981, 77, 341-348.	0.9	2
151	Impurity-induced tetramerization in Peierls-distorted polymers: Reducing the band gap. Solid State Communications, 1991, 77, 875-877.	0.9	2
152	Interaction energies between H ₂ O and HX \rightarrow CH=Y/X=CH \rightarrow YH for X, Y=CH ₂ , NH or O \rightarrow the chemical Hamiltonian approach. Chemical Physics Letters, 1991, 183, 25-30.	1.2	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.	0.7	2
155	A Note on the Symmetry Properties of Löwdin'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 two π -electron bonds to cold atoms. International Journal of Quantum Chemistry, 2013, 113, 185-189.	1.0	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 Lippmann-Schwinger equation. Molecular Physics, 2023, 121, .	0.8	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.	0.1	0
164	The high-rank Hartree-Fock method as an averaging procedure. Molecular Physics, 2006, 104, 2037-2046.	0.8	0
165	BSSE-free SCF methods for intermolecular interactions. International Journal of Quantum Chemistry, 1989, 36, 281-290.	1.0	0
166	Editorial: in memoriam János G. Ángyán (1956-2017). Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	0
167	On the variational principle for the non-linear Schrödinger equation. Journal of Mathematical Chemistry, 2020, 58, 340-351.	0.7	0
168	Comment on "Improved many-body expansions from eigenvector continuation": Physical Review C, 2021, 103, .	1.1	0
169	The γ function in quantum theory II. Mathematical challenges and paradoxa. Journal of Mathematical Chemistry, 2022, 60, 267-282.	0.7	0
170	Editorial: In memoriam István Mayer. International Journal of Quantum Chemistry, 2022, 122, .	1.0	0
171	A note on perturbation-adapted perturbation theory. Journal of Chemical Physics, 2022, 156, 116102.	1.2	0
172	Many-Body Perturbation Theory with Localized Orbitals: Accounting for Localization Diagrams as Integral Dressing. Journal of Chemical Theory and Computation, 2022, , .	2.3	0
173	Quantum chemical conformational analysis of the catalytic triad in β -chymotrypsin. Computational and Theoretical Chemistry, 1985, 24, 85-95.	1.5	0