

Josef Paldus

List of Publications by Year in descending order

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15,288
citations

14655

66
h-index

22832

112
g-index

258
all docs

258
docs citations

258
times ranked

2092
citing authors

#	ARTICLE	IF	CITATIONS
1	Correlation Problems in Atomic and Molecular Systems. IV. Extended Coupled-Pair Many-Electron Theory and Its Application to the BH ₃ Molecule. <i>Physical Review A</i> , 1972, 5, 50-67.	2.5	785
2	Stability Conditions for the Solutions of the Hartree-Fock Equations for Atomic and Molecular Systems. Application to the π -Electron Model of Cyclic Polyenes. <i>Journal of Chemical Physics</i> , 1967, 47, 3976-3985.	3.0	562
3	Correlation problems in atomic and molecular systems III. Rederivation of the coupled-pair many-electron theory using the traditional quantum chemical methods. <i>International Journal of Quantum Chemistry</i> , 1971, 5, 359-379.	2.0	533
4	Time-Independent Diagrammatic Approach to Perturbation Theory of Fermion Systems. <i>Advances in Quantum Chemistry</i> , 1975, 9, 105-197.	0.8	467
5	Group theoretical approach to the configuration interaction and perturbation theory calculations for atomic and molecular systems. <i>Journal of Chemical Physics</i> , 1974, 61, 5321-5330.	3.0	458
6	Applicability of coupled-pair theories to quasidegenerate electronic states: A model study. <i>International Journal of Quantum Chemistry</i> , 1980, 18, 1243-1269.	2.0	310
7	A Critical Assessment of Coupled Cluster Method in Quantum Chemistry. <i>Advances in Chemical Physics</i> , 2007, , 1-175.	0.3	285
8	Reduced multireference CCSD method: An effective approach to quasidegenerate states. <i>Journal of Chemical Physics</i> , 1997, 107, 6257-6269.	3.0	253
9	Correlation problems in atomic and molecular systems. V. Spin-adapted coupled cluster many-electron theory. <i>Journal of Chemical Physics</i> , 1977, 67, 303-318.	3.0	236
10	Spin-adapted multireference coupled-cluster approach: Linear approximation for two closed-shell-type reference configurations. <i>Journal of Chemical Physics</i> , 1988, 88, 5673-5687.	3.0	235
11	Application of Hilbert-space coupled-cluster theory to simple (H ₂) ₂ model systems: Planar models. <i>Physical Review A</i> , 1993, 47, 2738-2782.	2.5	217
12	Valence universal exponential ansatz and the cluster structure of multireference configuration interaction wave function. <i>Journal of Chemical Physics</i> , 1989, 90, 2714-2731.	3.0	214
13	Approximate account of the connected quadruply excited clusters in the coupled-pair many-electron theory. <i>Physical Review A</i> , 1984, 30, 2193-2209.	2.5	192
14	Stability Conditions for the Solutions of the Hartree-Fock Equations for Atomic and Molecular Systems. II. Simple Open-Shell Case. <i>Journal of Chemical Physics</i> , 1970, 52, 2919-2936.	3.0	170
15	Coupled Cluster Theory. <i>NATO ASI Series Series B: Physics</i> , 1992, , 99-194.	0.2	168
16	Automation of the implementation of spin-adapted open-shell coupled-cluster theories relying on the unitary group formalism. <i>Journal of Chemical Physics</i> , 1994, 101, 8812-8826.	3.0	160
17	Stability Conditions for the Solutions of the Hartree-Fock Equations for Atomic and Molecular Systems. VI. Singlet-Type Instabilities and Charge-Density-Wave Hartree-Fock Solutions for Cyclic Polyenes. <i>Physical Review A</i> , 1970, 2, 2268-2283.	2.5	158
18	Reduced multireference couple cluster method. II. Application to potential energy surfaces of HF, F ₂ , and H ₂ O. <i>Journal of Chemical Physics</i> , 1998, 108, 637-648.	3.0	158

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19	Cluster expansion analysis for delocalized systems. <i>International Journal of Quantum Chemistry</i> , 1969, 3, 149-167.	2.0	143
20	Coupled Cluster Approach. <i>Physica Scripta</i> , 1980, 21, 251-254.	2.5	143
21	General-model-space state-universal coupled-cluster theory: Connectivity conditions and explicit equations. <i>Journal of Chemical Physics</i> , 2003, 119, 5320-5333.	3.0	141
22	Unitary Group Approach to the Many-Electron Correlation Problem via Graphical Methods of Spin Algebras. <i>Physica Scripta</i> , 1980, 21, 295-311.	2.5	140
23	Clifford algebra and unitary group formulations of the many-electron problem. <i>Theoretica Chimica Acta</i> , 1988, 73, 81-103.	0.8	139
24	Correlation problems in atomic and molecular systems. VI. Coupled-cluster approach to open-shell systems. <i>Physical Review A</i> , 1978, 17, 805-815.	2.5	128
25	Time-dependent coupled cluster approach: Excitation energy calculation using an orthogonally spin-adapted formalism. <i>Journal of Chemical Physics</i> , 1986, 85, 1486-1501.	3.0	126
26	Unitary-group approach to the many-electron correlation problem: Relation of Gelfand and Weyl tableau formulations. <i>Physical Review A</i> , 1976, 14, 1620-1625.	2.5	123
27	Coupled cluster approach or quadratic configuration interaction?. <i>Journal of Chemical Physics</i> , 1989, 90, 4356-4362.	3.0	123
28	Orthogonally spin-adapted coupled-cluster equations involving singly and doubly excited clusters. Comparison of different procedures for spin-adaptation. <i>International Journal of Quantum Chemistry</i> , 1989, 36, 429-453.	2.0	118
29	Coupled-cluster approach to electron correlation in one dimension: Cyclic polyene model in delocalized basis. <i>Physical Review B</i> , 1984, 30, 4267-4291.	3.2	117
30	Orthogonally spin-adapted multi-reference Hilbert space coupled-cluster formalism: diagrammatic formulation. <i>Theoretica Chimica Acta</i> , 1992, 83, 69-103.	0.8	117
31	Orthogonally-spin-adapted coupled-cluster theory for closed-shell systems including triexcited clusters. <i>Physical Review A</i> , 1979, 20, 1-17.	2.5	116
32	Approximate account of connected quadruply excited clusters in single-reference coupled-cluster theory via cluster analysis of the projected unrestricted Hartree-Fock wave function. <i>Physical Review A</i> , 1996, 54, 1210-1241.	2.5	115
33	Orthogonally spin-adapted state-universal coupled-cluster formalism: Implementation of the complete two-reference theory including cubic and quartic coupling terms. <i>Journal of Chemical Physics</i> , 1994, 101, 5875-5890.	3.0	112
34	Doublet stability of ab initio SCF solutions for the allyl radical. <i>Molecular Physics</i> , 1978, 35, 445-459.	1.7	110
35	Application of graphical methods of spin algebras to limited CI approaches. I. Closed shell case. <i>International Journal of Quantum Chemistry</i> , 1977, 11, 813-848.	2.0	109
36	Coupled cluster approaches with an approximate account of triexcitations and the optimized inner projection technique. <i>Theoretica Chimica Acta</i> , 1990, 78, 65-128.	0.8	107

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37	Valence bond corrected single reference coupled cluster approach. <i>Theoretica Chimica Acta</i> , 1994, 89, 13-31.	0.8	107
38	Simultaneous handling of dynamical and nondynamical correlation via reduced multireference coupled cluster method: Geometry and harmonic force field of ozone. <i>Journal of Chemical Physics</i> , 1999, 110, 2844-2852.	3.0	102
39	Correlation effects in the low-lying excited states of the PPP models of alternant hydrocarbons. I. Qualitative rules for the effect of limited configuration interaction. <i>International Journal of Quantum Chemistry</i> , 1974, 8, 951-970.	2.0	100
40	An algebraic approach to bound states of simple one-electron systems. <i>International Journal of Quantum Chemistry</i> , 1977, 12, 875-896.	2.0	99
41	Stability Conditions for the Solutions of the Hartree-Fock Equations for Atomic and Molecular Systems. III. Rules for the Singlet Stability of Hartree-Fock Solutions of Electronic Systems. <i>Journal of Chemical Physics</i> , 1970, 53, 821-829.	3.0	98
42	Vectorizable approach to molecular CI problems using determinantal basis. <i>Chemical Physics Letters</i> , 1989, 155, 183-188.	2.6	98
43	Green's function approach to the direct perturbation calculation of the excitation energies of closed shell fermion systems. <i>Journal of Chemical Physics</i> , 1974, 60, 149-163.	3.0	96
44	Correlation problems in atomic and molecular systems. VII. Application of the open-shell coupled-cluster approach to simple π -electron model systems. <i>International Journal of Quantum Chemistry</i> , 1979, 15, 463-479.	2.0	92
45	Stability Conditions for the Solutions of the Hartree-Fock Equations for Atomic and Molecular Systems. IV. A Study of Doublet Stability for Odd Linear Polyenic Radicals. <i>Journal of Chemical Physics</i> , 1971, 54, 2293-2303.	3.0	91
46	Reduced multireference coupled cluster method: Rotational spectra of N ₂ . <i>Journal of Chemical Physics</i> , 2000, 113, 9966-9977.	3.0	91
47	Dissociation of N ₂ triple bond: a reduced multireference CCSD study. <i>Chemical Physics Letters</i> , 1998, 286, 145-154.	2.6	90
48	The general-model-space state-universal coupled-cluster method exemplified by the LiH molecule. <i>Journal of Chemical Physics</i> , 2003, 119, 5346-5357.	3.0	87
49	Externally corrected singles and doubles coupled cluster methods for open-shell systems. <i>Journal of Chemical Physics</i> , 1997, 107, 90-98.	3.0	86
50	Bond length alternation in cyclic polyenes. I. Restricted Hartree-Fock method. <i>International Journal of Quantum Chemistry</i> , 1983, 24, 373-394.	2.0	84
51	Clifford algebra unitary group approach to many-electron correlation problem. <i>Journal of Chemical Physics</i> , 1985, 83, 5135-5152.	3.0	84
52	Reduced multireference coupled cluster method with singles and doubles: Perturbative corrections for triples. <i>Journal of Chemical Physics</i> , 2006, 124, 174101.	3.0	84
53	Cluster analysis of the full configuration interaction wave functions of cyclic polyene models. <i>International Journal of Quantum Chemistry</i> , 1982, 22, 1281-1305.	2.0	81
54	Algebraic Approach to Coupled Cluster Theory. NATO ASI Series Series B: Physics, 1994, , 207-282.	0.2	80

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55	Molecular quadrupole moment functions of HF and N ₂ . I. Abinitio linear response coupled cluster results. <i>Journal of Chemical Physics</i> , 1996, 104, 4699-4715.	3.0	79
56	Relationship between configuration interaction and coupled cluster approaches. <i>Journal of Chemical Physics</i> , 1982, 76, 2458-2470.	3.0	78
57	Coupled-cluster approach to electron correlation in one dimension. II. Cyclic polyene model in localized basis. <i>Physical Review B</i> , 1985, 31, 5121-5142.	3.2	78
58	Energy versus amplitude corrected coupled-cluster approaches. II. Breaking the triple bond. <i>Journal of Chemical Physics</i> , 2001, 115, 5774-5783.	3.0	78
59	Unitary group approach to spin-adapted open-shell coupled cluster theory. <i>International Journal of Quantum Chemistry</i> , 1995, 56, 129-155.	2.0	75
60	Stability conditions for the solutions of the Hartree-Fock equations for the simple open-shell case. <i>Chemical Physics Letters</i> , 1969, 3, 1-3.	2.6	73
61	Applicability of valence universal multireference coupled cluster theories to quasidegenerate electronic states. I. Models involving at most two-body amplitudes. <i>Journal of Chemical Physics</i> , 1992, 97, 7600-7612.	3.0	72
62	Reduced multireference coupled cluster method IV: open-shell systems. <i>Molecular Physics</i> , 2000, 98, 1185-1199.	1.7	70
63	N-reference, M-state coupled-cluster method: Merging the state-universal and reduced multireference coupled-cluster theories. <i>Journal of Chemical Physics</i> , 2003, 119, 5334-5345.	3.0	69
64	Performance of the general-model-space state-universal coupled-cluster method. <i>Journal of Chemical Physics</i> , 2004, 120, 5890-5902.	3.0	69
65	Full potential energy curve for N ₂ by the reduced multireference coupled-cluster method. <i>Journal of Chemical Physics</i> , 2008, 129, 054104.	3.0	69
66	Applicability of multi-reference many-body perturbation theory to the determination of potential energy surfaces: A model study. <i>International Journal of Quantum Chemistry</i> , 1990, 38, 761-778.	2.0	66
67	Valence bond corrected single reference coupled cluster approach. <i>Theoretica Chimica Acta</i> , 1994, 89, 59-76.	0.8	66
68	Applicability of non-degenerate many-body perturbation theory to quasidegenerate electronic states: A model study. <i>International Journal of Quantum Chemistry</i> , 1983, 23, 1781-1802.	2.0	65
69	Coupled-cluster approaches with an approximate account of triexcitations and the optimized-inner-projection technique. II. Coupled-cluster results for cyclic-polyene model systems. <i>Physical Review B</i> , 1990, 42, 3351-3379.	3.2	65
70	Stability of Hartree-Fock solutions and symmetry breaking in the independent particle model: Abinitio case study of the LCAO-MO-SCF solutions for finite chains of hydrogen atoms. <i>Journal of Chemical Physics</i> , 1980, 72, 6546-6559.	3.0	64
71	Symmetry-adapted coupled-pair approach to the many-electron correlation problem. II. Application to the Be atom. <i>Physical Review A</i> , 1981, 24, 2316-2329.	2.5	61
72	Method of moments approach and coupled cluster theory. <i>Theoretica Chimica Acta</i> , 1991, 80, 223-243.	0.8	60

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73	General-model-space state-universal coupled-cluster methods for excited states: Diagonal noniterative triple corrections. <i>Journal of Chemical Physics</i> , 2006, 124, 034112.	3.0	60
74	Single-reference CCSD approach employing three- and four-body CAS SCF corrections: A preliminary study of a simple model. <i>International Journal of Quantum Chemistry</i> , 1997, 62, 137-151.	2.0	58
75	Unitary Group Approach to Many-Electron Correlation Problem. <i>Lecture Notes in Quantum Chemistry II</i> , 1981, , 1-50.	0.3	57
76	Symmetry-adapted coupled-pair approach to the many-electron correlation problem. III. Approximate coupled-pair approaches for the Be atom. <i>Physical Review A</i> , 1981, 24, 2330-2338.	2.5	56
77	Orthogonally spin-adapted single-reference coupled-cluster formalism: Linear response calculation of static properties. <i>Journal of Chemical Physics</i> , 1995, 102, 6511-6524.	3.0	55
78	Valence bond corrected single reference coupled cluster approach. <i>Theoretica Chimica Acta</i> , 1994, 89, 33-57.	0.8	54
79	Stability Conditions for the Solutions of the Hartree-Fock Equations for Atomic and Molecular Systems. V. The Nonanalytic Behavior of the Broken-Symmetry Solutions at the Branching Point. <i>Physical Review A</i> , 1971, 3, 525-527.	2.5	53
80	Spin-dependent unitary group approach. I. General formalism. <i>Journal of Chemical Physics</i> , 1990, 92, 7394-7401.	3.0	53
81	Bond length alternation in cyclic polyenes. VI. Coupled cluster approach with wannier orbital basis. <i>International Journal of Quantum Chemistry</i> , 1985, 28, 459-479.	2.0	52
82	The beginnings of coupled-cluster theory. , 2005, , 115-147.		52
83	A pattern calculus for the unitary group approach to the electronic correlation problem. <i>International Journal of Quantum Chemistry</i> , 1975, 9, 165-174.	2.0	52
84	Bond length alternation in cyclic polyenes. II. Unrestricted hartree-fock method. <i>International Journal of Quantum Chemistry</i> , 1983, 24, 395-409.	2.0	51
85	Alternancy symmetry: A unified viewpoint. <i>Journal of Chemical Physics</i> , 1985, 83, 1722-1735.	3.0	51
86	Applicability of nondegenerate many-body perturbation theory to quasi-degenerate electronic states. II. A two-state model. <i>International Journal of Quantum Chemistry</i> , 1985, 28, 525-534.	2.0	50
87	Clifford algebra unitary-group approach to many-electron system partitioning. <i>Physical Review A</i> , 1987, 35, 3197-3217.	2.5	50
88	Orthogonally spin-adapted single-reference coupled-cluster formalism: Linear response calculation of higher-order static properties. <i>Journal of Chemical Physics</i> , 1996, 104, 8566-8585.	3.0	50
89	Energy versus amplitude corrected coupled-cluster approaches. I. <i>Journal of Chemical Physics</i> , 2001, 115, 5759-5773.	3.0	49
90	Multi-reference Brillouin-Wigner coupled-cluster method with a general model space. <i>Molecular Physics</i> , 2005, 103, 2239-2245.	1.7	49

#	ARTICLE	IF	CITATIONS
91	Calculation of π -Band Positions of Aromatic Polycyclic Hydrocarbons by Limited Configuration Interaction Method. <i>Journal of Chemical Physics</i> , 1962, 36, 3129-3134.	3.0	48
92	Degeneracy and coupled-cluster approaches. <i>International Journal of Quantum Chemistry</i> , 1984, 26, 237-244.	2.0	48
93	Applicability of valence ϵ -universal multireference coupled ϵ -cluster theories to quasidegenerate electronic states. II. Models involving three ϵ -body amplitudes. <i>Journal of Chemical Physics</i> , 1994, 101, 3085-3095.	3.0	48
94	Coupled-Cluster approaches with an approximate account of triply and quadruply excited clusters: Implementation of the orthogonally spin-adapted CCD +ST(CCD), CCSD +T(CCSD), and ACPQ +ST(ACPQ) formalisms. <i>International Journal of Quantum Chemistry</i> , 1995, 55, 133-146.	2.0	48
95	Analysis of the multireference state-universal coupled-cluster Ansatz. <i>Journal of Chemical Physics</i> , 2003, 118, 6769-6783.	3.0	48
96	Lie Algebraic Approach to the Many-Electron Correlation Problem. <i>The IMA Volumes in Mathematics and Its Applications</i> , 1988, , 262-299.	0.5	47
97	Particle-hole formulation of the unitary group approach to the many-electron correlation problem. I. State construction and classification. <i>Physical Review A</i> , 1980, 22, 2299-2315.	2.5	46
98	Accounting for the exact degeneracy and quasidegeneracy in the automerization of cyclobutadiene via multireference coupled-cluster methods. <i>Journal of Chemical Physics</i> , 2009, 131, 114103.	3.0	46
99	Configuration interaction matrix elements. II. Graphical approach to the relationship between unitary group generators and permutations. <i>International Journal of Quantum Chemistry</i> , 1979, 16, 1321-1335.	2.0	45
100	Stability Conditions for Maximum-Overlap (Brueckner) Independent-Particle Wave Functions. <i>Physical Review A</i> , 1973, 8, 640-649.	2.5	44
101	Configuration interaction matrix elements. I. Algebraic approach to the relationship between unitary group generators and permutations. <i>International Journal of Quantum Chemistry</i> , 1979, 16, 1307-1319.	2.0	44
102	Particle-hole formulation of the unitary group approach to the many-electron correlation problem. II. Matrix element evaluation. <i>Physical Review A</i> , 1980, 22, 2316-2339.	2.5	44
103	Electron correlation in one dimension: Coupled cluster approaches to cyclic polyene π -electron models. <i>International Journal of Quantum Chemistry</i> , 1992, 42, 135-164.	2.0	43
104	Comparison of the open ϵ -shell state ϵ -universal and state ϵ -selective coupled ϵ -cluster theories: H4 and H8 models. <i>Journal of Chemical Physics</i> , 1995, 103, 1024-1034.	3.0	43
105	Singlet-Triplet Splitting in Methylene: An Accurate Description of Dynamic and Nondynamic Correlation by Reduced Multireference Coupled Cluster Method. <i>Collection of Czechoslovak Chemical Communications</i> , 1998, 63, 1381-1393.	1.0	43
106	A truncated version of reduced multireference coupled-cluster method with singles and doubles and noniterative triples: Application to F2 and Ni(CO) $_n$ ($n=1, 2,$ and 4). <i>Journal of Chemical Physics</i> , 2006, 125, 164107.	3.0	43
107	Representation theory of $so(4,2)$ for the perturbation treatment of hydrogenic-type hamiltonians by algebraic methods. <i>International Journal of Quantum Chemistry</i> , 1982, 21, 153-171.	2.0	42
108	Truncated version of the reduced multireference coupled-cluster method with perturbation selection of higher than pair clusters. <i>International Journal of Quantum Chemistry</i> , 2000, 80, 743-756.	2.0	42

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109	Bond length alternation in cyclic polyenes. IV. Finite-order perturbation theory approach. <i>International Journal of Quantum Chemistry</i> , 1984, 25, 423-443.	2.0	41
110	Perturbation theory and electron correlation in extended systems: Cyclic polyene model. <i>International Journal of Quantum Chemistry</i> , 1983, 24, 707-727.	2.0	40
111	Spin-adapted open-shell state-selective coupled cluster approach and doublet stability of its Hartree-Fock reference. <i>Journal of Chemical Physics</i> , 1995, 102, 2013-2023.	3.0	40
112	Singlet-triplet separation in BN and C2: Simple yet exceptional systems for advanced correlated methods. <i>Chemical Physics Letters</i> , 2006, 431, 179-184.	2.6	40
113	Quasi-degeneracy and coupled-pair theories. <i>Chemical Physics Letters</i> , 1979, 67, 144-148.	2.6	39
114	On the solution of coupled-cluster equations in the fully correlated limit of cyclic polyene model. <i>International Journal of Quantum Chemistry</i> , 1991, 40, 9-34.	2.0	39
115	Energy- versus amplitude-corrected coupled-cluster approaches. III. Accurate computation of spectroscopic data exemplified on the HF molecule. <i>Journal of Chemical Physics</i> , 2002, 117, 1941-1955.	3.0	39
116	The instabilities of the Hartree-Fock solutions for cyclic polyenes with respect to the spin and charge density fluctuations. <i>Journal of Polymer Science Part C Polymer Symposia</i> , 1970, 29, 199-210.	0.1	39
117	Symmetry Breaking in the Independent Particle Model. , 2003, , 67-139.		39
118	Application of graphical methods of spin algebras to limited CI approaches. II. A simple open shell case. <i>International Journal of Quantum Chemistry</i> , 1977, 11, 849-867.	2.0	38
119	Valence bond approach to the Pariser-Parr-Pople Hamiltonian and its application to simple π -electron systems. <i>Computational and Theoretical Chemistry</i> , 1991, 229, 249-278.	1.5	38
120	Size extensivity of a general-model-space state-universal coupled-cluster method. <i>International Journal of Quantum Chemistry</i> , 2004, 99, 914-924.	2.0	38
121	Multireference general-model-space state-universal and state-specific coupled-cluster approaches to excited states. <i>Journal of Chemical Physics</i> , 2010, 133, 184106.	3.0	38
122	Hartree-Fock stability and symmetry breaking: oxygen doubly negative ion. <i>Canadian Journal of Chemistry</i> , 1985, 63, 1803-1811.	1.1	37
123	Unitary group based state-selective coupled-cluster method: Comparison of the first order interacting space and the full single and double excitation space approximations. <i>Journal of Chemical Physics</i> , 1995, 102, 8897-8905.	3.0	37
124	Real or artifactual symmetry breaking in the BNB radical: A multireference coupled cluster viewpoint. <i>Journal of Chemical Physics</i> , 2007, 126, 224304.	3.0	37
125	A unitary group based open-shell coupled cluster study of vibrational frequencies in ground and excited states of first row diatomics. <i>Journal of Chemical Physics</i> , 1996, 104, 9555-9562.	3.0	36
126	Multireference Coupled-Cluster Methods: Recent Developments. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2010, , 455-489.	0.6	36

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127	Valence bond approach exploiting Clifford algebra realization of Rumer-Weyl basis. <i>International Journal of Quantum Chemistry</i> , 1992, 41, 117-146.	2.0	35
128	Externally corrected singles and doubles coupled cluster methods for open-shell systems. II. Applications to the low lying doublet states of OH, NH ₂ , CH ₃ and CN radicals. <i>Molecular Physics</i> , 1998, 94, 235-248.	1.7	35
129	Bond length alternation in cyclic polyenes. V. Local finite-order perturbation theory approach. <i>International Journal of Quantum Chemistry</i> , 1984, 26, 349-371.	2.0	34
130	Coupled cluster approach or quadratic configuration interaction?: Reply to comment by Pople, Head-Gordon, and Raghavachari. <i>Journal of Chemical Physics</i> , 1990, 93, 1485-1486.	3.0	34
131	Correlation effects in the low-lying excited states of the PPP models of alternant hydrocarbons. II. State correlation diagrams. <i>International Journal of Quantum Chemistry</i> , 1974, 8, 293-303.	2.0	34
132	A Comment on the Paper by Hideo Fukutome: Spin Density Wave and Charge Transfer Wave in Long Conjugated Molecules. <i>Progress of Theoretical Physics</i> , 1969, 42, 769-774.	2.0	33
133	Bond length alternation in cyclic polyenes. III. Alternant molecular orbital method. <i>International Journal of Quantum Chemistry</i> , 1983, 24, 411-423.	2.0	33
134	Spin properties of radicaloid alternant hydrocarbons. Exact solutions for representative Pariser-Parr-Pople model systems. <i>Journal of Chemical Physics</i> , 1984, 80, 2244-2246.	3.0	33
135	Unitary group approach to reduced density matrices. <i>Journal of Chemical Physics</i> , 1990, 93, 4142-4153.	3.0	33
136	Symmetry-adapted coupled-pair approach to the many-electron correlation problem. I. LS-adapted theory for closed-shell atoms. <i>Physical Review A</i> , 1981, 24, 2302-2315.	2.5	32
137	Study of the correlation effects in a three-electron model system using the projected Hartree-Fock method and the natural spin orbital formalism. <i>Journal of Chemical Physics</i> , 1973, 59, 2560-2571.	3.0	31
138	A remark on doublet stability of allyl radical restricted SCF solutions. <i>Chemical Physics Letters</i> , 1977, 50, 6-8.	2.6	31
139	Perturbatively selected CI as an optimal source for externally corrected CCSD. <i>Journal of Chemical Physics</i> , 1999, 110, 11708-11716.	3.0	31
140	Electron Correlation in Small Molecules: Grafting CI onto CC. <i>Topics in Current Chemistry</i> , 1999, , 1-20.	4.0	31
141	Multiconfigurational spin-adapted single-reference coupled cluster formalism. <i>International Journal of Quantum Chemistry</i> , 1993, 48, 269-285.	2.0	30
142	Unitary group based state specific open-shell singlet coupled cluster method: Application to ozone and comparison with Hilbert and Fock space theories. <i>Journal of Chemical Physics</i> , 1995, 102, 8059-8070.	3.0	30
143	Partially linearized, fully size-extensive, and reduced multireference coupled-cluster methods. II. Applications and performance. <i>Journal of Chemical Physics</i> , 2008, 128, 144119.	3.0	30
144	Convergence of the Rayleigh-Schrödinger perturbation expansions for the energy levels of the Pariser-Parr-Pople model of the benzene molecule. <i>Journal of Chemical Physics</i> , 1974, 60, 4825-4829.	3.0	29

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145	Model space incompleteness in multireference state-universal and state-selective coupled-cluster theories. <i>Chemical Physics Letters</i> , 2010, 496, 183-187.	2.6	29
146	Externally and internally corrected coupled cluster approaches: an overview. <i>Journal of Mathematical Chemistry</i> , 2017, 55, 477-502.	1.5	29
147	Calculation of permutation matrices using graphical methods of spin algebras: Explicit expressions for the Serber-coupling case. <i>Physical Review A</i> , 1978, 18, 827-840.	2.5	28
148	Clifford algebra realization of Rumer-Weyl basis. <i>Computational and Theoretical Chemistry</i> , 1989, 199, 85-101.	1.5	27
149	Unitary group based open-shell coupled cluster approach and triplet and open-shell singlet stabilities of Hartree-Fock references. <i>Journal of Chemical Physics</i> , 1995, 103, 6536-6547.	3.0	27
150	On the significance of quadruply excited clusters in coupled-cluster calculations for the low-lying states of BN and C . <i>Chemical Physics Letters</i> , 2008, 461, 321-326.	2.6	26
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