Josef Paldus

List of Publications by Year in descending order

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254 papers 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	Matrix elements of unitary group generators in many-fermion correlation problem. II. Graphical methods of spin algebras. Journal of Mathematical Chemistry, 2021, 59, 37-71.	1.5	10
2	Matrix elements of unitary group generators in many-fermion correlation problem. III. Green-Gould approach. Journal of Mathematical Chemistry, 2021, 59, 72-118.	1.5	3
3	Matrix elements of unitary group generators in many-fermion correlation problem. I. tensorial approaches. Journal of Mathematical Chemistry, 2021, 59, 1-36.	1.5	12
4	Valence bond approach and Verma bases. Journal of Mathematical Chemistry, 2018, 56, 1595-1630.	1.5	3
5	Externally and internally corrected coupled cluster approaches: an overview. Journal of Mathematical Chemistry, 2017, 55, 477-502.	1.5	29
6	Multireference coupled-cluster approaches to excited states. , 2015, , .		1
7	On the cluster structure of linear-chain fermionic wave functions. Journal of Mathematical Chemistry, 2015, 53, 629-650.	1.5	1
8	CCSD(T) calculations of confined systems: In-crystal polarizabilities of Fâ^', Clâ^', O2 â^', and S2 â^'. Journal of Chemical Physics, 2014, 141, 214303.	3.0	16
9	Unitary group approach to the many-electron correlation problem: spin-dependent operators. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	7
10	Symmetry-breaking in the independent particle model: nature of the singular behavior of Hartree–Fock potentials. Journal of Mathematical Chemistry, 2013, 51, 427-450.	1.5	1
11	Multi-reference state-universal coupled-cluster approaches to electronically excited states. Journal of Chemical Physics, 2011, 134, 214118.	3.0	23
12	Multireference coupled-cluster study of the symmetry breaking in the C2B radical. Journal of Chemical Physics, 2011, 134, 074301.	3.0	4
13	Model space incompleteness in multireference state-universal and state-selective coupled-cluster theories. Chemical Physics Letters, 2010, 496, 183-187.	2.6	29
14	Multireference coupledâ€cluster methods for ground and lowâ€lying excited states. A benchmark illustration on CH ⁺ potentials. International Journal of Quantum Chemistry, 2010, 110, 2734-2743.	2.0	13
15	Multireference Coupled-Cluster Methods: Recent Developments. Challenges and Advances in Computational Chemistry and Physics, 2010, , 455-489.	0.6	36
16	QCI and related CC approaches: a retrospection. Molecular Physics, 2010, 108, 2941-2950.	1.7	10
17	Performance of multireference and equation-of-motion coupled-cluster methods for potential energy surfaces of low-lying excited states: Symmetric and asymmetric dissociation of water. Journal of Chemical Physics, 2010, 133, 024102.	3.0	8
18	Multireference general-model-space state-universal and state-specific coupled-cluster approaches to excited states. Journal of Chemical Physics, 2010, 133, 184106.	3.0	38

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19	A Multireference Coupled-Cluster Study of Electronic Excitations in Furan and Pyrrole ^{â€} . Journal of Physical Chemistry A, 2010, 114, 8591-8600.	2.5	23
20	Accounting for the exact degeneracy and quasidegeneracy in the automerization of cyclobutadiene via multireference coupled-cluster methods. Journal of Chemical Physics, 2009, 131, 114103.	3.0	46
21	Symmetry breaking in spinâ€restricted, openâ€shell Hartree–Fock wave functions. International Journal of Quantum Chemistry, 2009, 109, 1756-1765.	2.0	10
22	Energetics of 1, <i>n</i> i>â€didehydroâ€polyene diradicals and performance of reduced multireference coupledâ€cluster method. International Journal of Quantum Chemistry, 2009, 109, 3305-3314.	2.0	5
23	Symmetry breaking in spin-restricted Hartree–Fock solutions: the case of the C2 molecule and the N2+ and F2+ cations. Physical Chemistry Chemical Physics, 2009, 11, 5281.	2.8	17
24	Do independent-particle-model broken-symmetry solutions contain more physics than the symmetry-adapted ones? The case of homonuclear diatomics. Journal of Chemical Physics, 2009, 130, 084110.	3.0	21
25	The Energy Level Structure of Low-dimensional Multi-electron Quantum Dots. Advances in Quantum Chemistry, 2009, , 177-201.	0.8	15
26	Analysis and classification of symmetry breaking in linear ABA-type triatomics. Journal of Chemical Physics, 2009, 130, 164116.	3.0	8
27	Approximate symmetry-breaking in the independent particle model of monocyclic completely conjugated polyenes. Journal of Mathematical Chemistry, 2008, 44, 88-120.	1.5	9
28	Coupledâ€cluster approach to spontaneous symmetry breaking in molecules: The linear N ₃ radical. International Journal of Quantum Chemistry, 2008, 108, 2117-2127.	2.0	14
29	On the significance of quadruply excited clusters in coupled-cluster calculations for the low-lying states of BN and <mml:math altimg="si70.gif" display="inline" overflow="scroll" xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow><mml:mrow< td=""><td>2.6 ow><mml:r< td=""><td>26 nn>2</td></mml:r<></td></mml:mrow<></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:mrow></mml:msub></mml:mrow></mml:math>	2. 6 ow> <mml:r< td=""><td>26 nn>2</td></mml:r<>	26 nn>2
30	Independent particle model of spontaneous symmetry breaking in planar π-electron systems. European Physical Journal D, 2008, 46, 453-461.	1.3	4
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32	REDUCED MULTIREFERENCE COUPLED-CLUSTER METHOD AND ITS APPLICATION TO THE PYRIDYNE DIRADICALS. Journal of Theoretical and Computational Chemistry, 2008, 07, 805-820.	1.8	18
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35	Nondynamic Correlation and Coupled-Cluster Methods. AIP Conference Proceedings, 2008, , .	0.4	0
36	Binding in transition metal complexes: Reduced multireference coupled-cluster study of the MCH2+ (M=Sc to Cu) compounds. Journal of Chemical Physics, 2007, 126, 234303.	3.0	24

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37	Real or artifactual symmetry breaking in the BNB radical: A multireference coupled cluster viewpoint. Journal of Chemical Physics, 2007, 126, 224304.	3.0	37
38	A Critical Assessment of Coupled Cluster Method in Quantum Chemistry. Advances in Chemical Physics, 2007, , 1-175.	0.3	285
39	Reduced Multireference Coupled-Cluster Method:  Barrier Heights for Heavy Atom Transfer, Nucleophilic Substitution, Association, and Unimolecular Reactions. Journal of Physical Chemistry A, 2007, 111, 11189-11197.	2.5	16
40	Hartree-Fock Stability and Broken Symmetry Solutions of O2- and S2- Anions in External Confinement. Collection of Czechoslovak Chemical Communications, 2007, 72, 197-222.	1.0	10
41	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). Journal of Chemical Physics, 2006, 125, 164107.	3.0	43
42	General-model-space state-universal coupled-cluster methods for excited states: Diagonal noniterative triple corrections. Journal of Chemical Physics, 2006, 124, 034112.	3.0	60
43	Reduced multireference coupled cluster method with singles and doubles: Perturbative corrections for triples. Journal of Chemical Physics, 2006, 124, 174101.	3.0	84
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45	General-model-space state-universal coupled-cluster method: excitation energies of water. Molecular Physics, 2006, 104, 661-676.	1.7	25
46	Singlet–triplet separation in BN and C2: Simple yet exceptional systems for advanced correlated methods. Chemical Physics Letters, 2006, 431, 179-184.	2.6	40
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48	Diagonal perturbative triple corrections to the general-model-space state-universal coupled-cluster method: are they warranted and useful?. Molecular Physics, 2006, 104, 2047-2062.	1.7	16
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52	Can We Avoid the Intruder-State Problems in the State-Universal Coupled-Cluster Approaches While Preserving Size Extensivity?. Collection of Czechoslovak Chemical Communications, 2004, 69, 90-104.	1.0	24
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55	Performance of the general-model-space state-universal coupled-cluster method. Journal of Chemical Physics, 2004, 120, 5890-5902.	3.0	69
56	General-model-space state-universal coupled-cluster theory: Connectivity conditions and explicit equations. Journal of Chemical Physics, 2003, 119, 5320-5333.	3.0	141
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60	COUPLED-CLUSTER APPROACH TO CORRELATION IN SMALL MOLECULES: ENERGY VERSUS AMPLITUDE CORRECTED METHODS. International Journal of Modern Physics B, 2003, 17, 5379-5391.	2.0	3
61	Symmetry Breaking in the Independent Particle Model. , 2003, , 67-139.		39
62	Simultaneous Account of Dynamic and Nondynamic Correlations Based on Complementarity of CI and CC Approaches. ACS Symposium Series, 2002, , 10-30.	0.5	12
63	Energy- versus amplitude-corrected coupled-cluster approaches. III. Accurate computation of spectroscopic data exemplified on the HF molecule. Journal of Chemical Physics, 2002, 117, 1941-1955.	3.0	39
64	COUPLED-CLUSTER APPROACH TO CORRELATION IN SMALL MOLECULES: ENERGY $\langle i \rangle VS. \langle i \rangle$ AMPLITUDE CORRECTED METHODS., 2002, , .		0
65	Energy versus amplitude corrected coupled-cluster approaches. I. Journal of Chemical Physics, 2001, 115, 5759-5773.	3.0	49
66	Energy versus amplitude corrected coupled-cluster approaches. II. Breaking the triple bond. Journal of Chemical Physics, 2001, 115, 5774-5783.	3.0	78
67	Approximate Coupled Cluster Methods: Combined Reduced Multireference and Almost–Linear Coupled Cluster Methods with Singles and Doubles 11This paper is dedicated to Professor Giuseppe Del Re at the occasion of his 65th anniversary Advances in Quantum Chemistry, 2000, 36, 231-251.	0.8	18
68	Algebraic solutions for point groups: Cubic groupsG in the group chainG?T?D2?C2. International Journal of Quantum Chemistry, 2000, 76, 585-599.	2.0	5
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71	Truncated version of the reduced multireference coupled-cluster method with perturbation selection of higher than pair clusters. International Journal of Quantum Chemistry, 2000, 80, 743-756.	2.0	42
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74	Reduced multireference coupled cluster method IV: open-shell systems. Molecular Physics, 2000, 98, 1185-1199.	1.7	70
75	Reduced multireference coupled cluster method: Ro-vibrational spectra of N2. Journal of Chemical Physics, 2000, 113, 9966-9977.	3.0	91
76	Direct iterative solution of the generalized Bloch equation. II. A general formalism for many-electron systems. Journal of Chemical Physics, 2000, 113, 2594-2611.	3.0	19
77	Direct iterative solution of the generalized Bloch equation. IV. Application to H2, LiH, BeH, and CH2. Journal of Chemical Physics, 2000, 113, 2622-2637.	3.0	21
78	Direct iterative solution of the generalized Bloch equation. III. Application to H2-cluster models. Journal of Chemical Physics, 2000, 113, 2612-2621.	3.0	15
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80	Perturbatively selected CI as an optimal source for externally corrected CCSD. Journal of Chemical Physics, 1999, 110, 11708-11716.	3.0	31
81	Size dependence of theX1Ag?11Bu excitation energy in linear polyenes. International Journal of Quantum Chemistry, 1999, 74, 177-192.	2.0	12
82	Electron Correlation in Small Molecules: Grafting CI onto CC. Topics in Current Chemistry, 1999, , 1-20.	4.0	31
83	Simultaneous handling of dynamical and nondynamical correlation via reduced multireference coupled cluster method: Geometry and harmonic force field of ozone. Journal of Chemical Physics, 1999, 110, 2844-2852.	3.0	102
84	Dissociation of N2 triple bond: a reduced multireference CCSD study. Chemical Physics Letters, 1998, 286, 145-154.	2.6	90
85	Unitary-group-based open-shell coupled-cluster method with corrections for connected triexcited clusters. I. Theory. International Journal of Quantum Chemistry, 1998, 70, 65-75.	2.0	10
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89	Unitary group based open-shell coupled cluster method with corrections for connected triexcited clusters. II. Applications. Molecular Physics, 1998, 94, 41-54.	1.7	14
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91	Externally corrected singles and doubles coupled cluster methods for open-shell systems. Journal of Chemical Physics, 1997, 107, 90-98.	3.0	86
92	UNITARY GROUP BASED COUPLED CLUSTER METHODS AND CALCULATION OF MOLECULAR PROPERTIES. Recent Advances in Computational, 1997 , , $183-219$.	0.8	14
93	Title is missing!. Journal of Mathematical Chemistry, 1997, 21, 51-70.	1.5	13
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100	Molecular quadrupole moment function of ammonia. Journal of Chemical Physics, 1996, 105, 11068-11074.	3.0	18
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108	Orthogonally spinâ€adapted singleâ€reference coupledâ€cluster formalism: Linear response calculation of static properties. Journal of Chemical Physics, 1995, 102, 6511-6524.	3.0	55

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110	Unitary group based state specific openâ€shellâ€singlet coupledâ€cluster method: Application to ozone and comparison with Hilbert and Fock space theories. Journal of Chemical Physics, 1995, 102, 8059-8070.	3.0	30
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