Hans-Joachim Werner

List of Publications by Year
in descending order

310	53,429	1888	1253
papers	citations	102 h-index	226 g-index

322	322	322	11459
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	An efficient internally contracted multiconfigurationâ€“reference configuration interaction method. Journal of Chemical Physics, 1988, 89, 5803-5814.	1.2	3,487
2	Molpro: a generalâ€purpose quantum chemistry program package. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 242-253.	6.2	2,852
3	A second order multiconfiguration SCF procedure with optimum convergence. Journal of Chemical Physics, 1985, 82, 5053-5063.	1.2	2,827
4	An efficient method for the evaluation of coupling coefficients in configuration interaction calculations. Chemical Physics Letters, 1988, 145, 514-522.	1.2	2,534
5	An efficient second-order MC SCF method for long configuration expansions. Chemical Physics Letters, 1985, 115, 259-267.	1.2	2,454
6	Coupled cluster theory for high spin, open shell reference wave functions. Journal of Chemical Physics, 1993, 99, 5219-5227.	1.2	1,878
7	A simple and efficient CCSD(T)-F12 approximation. Journal of Chemical Physics, 2007, 127, 221106.	1.2	1,587
8	A comparison of the efficiency and accuracy of the quadratic configuration interaction (QCISD), coupled cluster (CCSD), and Brueckner coupled cluster (BCCD) methods. Chemical Physics Letters, 1992, 190, 1-12.	1.2	1,561
9	Simplified CCSD(T)-F12 methods: Theory and benchmarks. Journal of Chemical Physics, 2009, 130, 054104.	1.2	1,558
10	Systematically convergent basis sets for explicitly correlated wavefunctions: The atoms H, He, Bâ€“Ne, and Alâ€“Ar. Journal of Chemical Physics, 2008, 128, 084102.	1.2	1,115
11	Spin-orbit matrix elements for internally contracted multireference configuration interaction wavefunctions. Molecular Physics, 2000, 98, 1823-1833.	0.8	856
12	Multireference perturbation theory for large restricted and selected active space reference wave functions. Journal of Chemical Physics, 2000, 112, 5546-5557.	1.2	791
13	Local treatment of electron correlation in coupled cluster theory. Journal of Chemical Physics, 1996, 104, 6286-6297.	1.2	703
14	Combining long-range configuration interaction with short-range density functionals. Chemical Physics Letters, 1997, 275, 151-160.	1.2	681
15	Low-order scaling local electron correlation methods. I. Linear scaling local MP2. Journal of Chemical Physics, 1999, 111, 5691-5705.	1.2	671
16	Fast linear scaling second-order MÃ¸ller-Plesset perturbation theory (MP2) using local and density fitting approximations. Journal of Chemical Physics, 2003, 118, 8149-8160.	1.2	652
17	PNO-CI and PNO-CEPA studies of electron correlation effects. Molecular Physics, 1976, 31, 855-872.	0.8	621
18	The Molpro quantum chemistry package. Journal of Chemical Physics, 2020, 152, 144107.	1.2	603

#	Article	IF	Citations
19	Low-order scaling local electron correlation methods. IV. Linear scaling local coupled-cluster (LCCSD). Journal of Chemical Physics, 2001, 114, 661.	1.2	564
20	Third-order multireference perturbation theory The CASPT3 method. Molecular Physics, 1996, 89, 645-661.	0.8	545
21	Internally contracted multiconfiguration-reference configuration interaction calculations for excited states. Theoretica Chimica Acta, 1992, 84, 95-103.	0.9	504
22	General orbital invariant MP2-F12 theory. Journal of Chemical Physics, 2007, 126, 164102.	1.2	490
23	A quadratically convergent MCSCF method for the simultaneous optimization of several states. Journal of Chemical Physics, 1981, 74, 5794-5801.	1.2	450
24	An accurate multireference configuration interaction calculation of the potential energy surface for the F+H2â†'HF+H reaction. Journal of Chemical Physics, 1996, 104, 6515-6530.	1.2	382
25	The selfâ€consistent electron pairs method for multiconfiguration reference state functions. Journal of Chemical Physics, 1982, 76, 3144-3156.	1.2	375
26	Communication: Extended multi-state complete active space second-order perturbation theory: Energy and nuclear gradients. Journal of Chemical Physics, 2011, 135, 081106.	1.2	374
27	A quadratically convergent multiconfigurationâ€"selfâ€consistent field method with simultaneous optimization of orbitals and CI coefficients. Journal of Chemical Physics, 1980, 73, 2342-2356.	1.2	331
28	Finite perturbation calculations for the static dipole polarizabilities of the first-row atoms. Physical Review A, 1976, 13, 13-16.	1.0	311
29	MCSCF study of the avoided curve crossing of the two lowest 1Î£+ states of LiF. Journal of Chemical Physics, 1981, 74, 5802-5807.	1.2	310
30	Local perturbative triples correction (T) with linear cost scaling. Chemical Physics Letters, 2000, 318, 370-378.	1.2	296
31	van der Waals Interactions in the Cl + HD Reaction. Science, 1999, 286, 1713-1716.	6.0	287
32	Magnetic Field Dependence of the Geminate Recombination of Radical Ion Pairs in Polar Solvents. Zeitschrift Fur Physikalische Chemie, 1976, 101, 371-390.	1.4	278
33	Fast Hartreeâ€"Fock theory using local density fitting approximations. Molecular Physics, 2004, 102, 2311-2321.	0.8	276
34	Local treatment of electron excitations in the EOM-CCSD method. Journal of Chemical Physics, 2003, 118, 3006-3019.	1.2	273
35	The Transition State of the F + H2 Reaction. Science, 1993, 262, 1852-1855.	6.0	256
36	High-Accuracy Computation of Reaction Barriers in Enzymes. Angewandte Chemie - International Edition, 2006, 45, 6856-6859.	7.2	253

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37	Extrapolating MP2 and CCSD explicitly correlated correlation energies to the complete basis set limit with first and second row correlation consistent basis sets. Journal of Chemical Physics, 2009, 131, 194105.	1.2	251
38	Analytical energy gradients for internally contracted second-order multireference perturbation theory. Journal of Chemical Physics, 2003, 119, 5044-5057.	1.2	248
39	A new internally contracted multi-reference configuration interaction method. Journal of Chemical Physics, 2011, 135, 054101.	1.2	246
40	An efficient local coupled cluster method for accurate thermochemistry of large systems. Journal of Chemical Physics, 2011, 135, 144116.	1.2	244
41	Explicitly correlated RMP2 for high-spin open-shell reference states. Journal of Chemical Physics, 2008, 128, 154103.	1.2	242
42	An investigation of the F+H2 reaction based on a full ab initio description of the open-shell character of the F(2P) atom. Journal of Chemical Physics, 2000, 113, 11084-11100.	1.2	238
43	First-Principles Theory for the H + CH4 -> H2 + CH3 Reaction. Science, 2004, 306, 2227-2229.	6.0	238
44	Quantum mechanical angular distributions for the F+H2 reaction. Journal of Chemical Physics, 1996, 104, 6531-6546.	1.2	232
45	Local Treatment of Electron Correlation in Molecular Clusters:Â Structures and Stabilities of (H2O)n,n= 2â^'4. Journal of Physical Chemistry A, 1998, 102, 5997-6003.	1.1	231
46	Explicitly correlated multireference configuration interaction: MRCI-F12. Journal of Chemical Physics, 2011, 134, 034113.	1.2	223
47	Analytical energy gradients for local second-order MÃ¸llerâ€“Plesset perturbation theory using density fitting approximations. Journal of Chemical Physics, 2004, 121, 737-750.	1.2	220
48	Calculation of intermolecular interactions in the benzene dimer using coupled-cluster and local electron correlation methods. Physical Chemistry Chemical Physics, 2006, 8, 4072.	1.3	211
49	Adiabatic and diabatic potential energy surfaces for collisions of CN(Xâ€‰2Î£+,â€‰Aâ€‰2Î) with He. Journal of Chemical Physics, 1988, 89, 3139-3151.	1.2	208
50	Matrix-Formulated Direct Multiconfiguration Self-Consistent Field and Multiconfiguration Reference Configuration-Interaction Methods. Advances in Chemical Physics, 2007, , 1-62.	0.3	205
51	Analytical energy gradients for local second-order Mo/llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 1998, 108, 5185-5193.	1.2	204
52	Low-order scaling local correlation methods II: Splitting the Coulomb operator in linear scaling local second-order MÃ¸llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 2000, 113, 9443-9455.	1.2	201
53	Explicitly correlated coupled cluster methods with pair-specific geminals. Molecular Physics, 2011, 109, 407-417.	0.8	200
54	Molecular properties from MCSCFâ€SCEP wave functions. I. Accurate dipole moment functions of OH, OHâ^', and OH+. Journal of Chemical Physics, 1983, 79, 905-916.	1.2	193

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55	Characterization of theS1â€“S2conical intersection in pyrazine usingabinitiomulticonfiguration selfâ€consistentâ€field and multireference configurationâ€interaction methods. Journal of Chemical Physics, 1994, 100, 1400-1413.	1.2	193
56	A short-range gradient-corrected density functional in long-range coupled-cluster calculations for rare gas dimers. Physical Chemistry Chemical Physics, 2005, 7, 3917.	1.3	192
57	Multipole approximation of distant pair energies in local MP2 calculations. Chemical Physics Letters, 1998, 290, 143-149.	1.2	184
58	A comparison of variational and non-variational internally contracted multiconfiguration-reference configuration interaction calculations. Theoretica Chimica Acta, 1991, 78, 175-187.	0.9	175
59	Accurate calculation of vibrational frequencies using explicitly correlated coupled-cluster theory. Journal of Chemical Physics, 2009, 130, 054105.	1.2	173
60	Theory of the magnetic field modulated geminate recombination of radical ion pairs in polar solvents: Application to the pyreneâ€“N,Nâ€dimethylaniline system. Journal of Chemical Physics, 1977, 67, 646-663.	1.2	163
61	The aurophilic attraction as interpreted by local correlation methods. Journal of Chemical Physics, 1999, 110, 7210-7215.	1.2	163
62	The orbital-specific-virtual local coupled cluster singles and doubles method. Journal of Chemical Physics, 2012, 136, 144105.	1.2	163
63	Local explicitly correlated second-order perturbation theory for the accurate treatment of large molecules. Journal of Chemical Physics, 2009, 130, 054106.	1.2	160
64	Photodissociation dynamics of H2S on new coupled ab initio potential energy surfaces. Journal of Chemical Physics, 1999, 111, 4523-4534.	1.2	159
65	Dynamically weighted multiconfiguration self-consistent field: Multistate calculations for F+H2Oâ†'HF+OH reaction paths. Journal of Chemical Physics, 2004, 120, 7281-7289.	1.2	153
66	Third-order multireference perturbation theory The CASPT3 method. Molecular Physics, 1996, 89, 645-661.	0.8	153
67	TheAâ€‰2Îâ€“Xâ€‰2Î£+red andBâ€‰2Î£+â€“Xâ€‰2Î£+violet systems of the CN radical: Accurate multireference configuration interaction calculations of the radiative transition probabilities. Journal of Chemical Physics, 1988, 89, 7334-7343.	1.2	151
68	Explicitly correlated local coupledâ€cluster methods using pair natural orbitals. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1371.	6.2	151
69	Accurate Calculations of Intermolecular Interaction Energies Using Explicitly Correlated Coupled Cluster Wave Functions and a Dispersion-Weighted MP2 Method. Journal of Physical Chemistry A, 2009, 113, 11580-11585.	1.1	150
70	Breakdown of the Born-Oppenheimer Approximation in the F+ o -D ₂ â†' DF + D Reaction. Science, 2007, 317, 1061-1064.	6.0	149
71	Local explicitly correlated coupled-cluster methods: Efficient removal of the basis set incompleteness and domain errors. Journal of Chemical Physics, 2009, 130, 241101.	1.2	149
72	Multireference configuration interaction calculations of the lowâ€lying electronic states of ClO2. Journal of Chemical Physics, 1992, 96, 8948-8961.	1.2	144

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73	Ab initio geometry optimization for large molecules. Journal of Computational Chemistry, 1997, 18, 1473-1483.	1.5	144
74	Theoretical dipole moment functions of the HF, HCl, and HBr molecules. Journal of Chemical Physics, 1980, 73, 2319-2328.	1.2	140
75	Global ab initio potential energy surfaces for the ClH2 reactive system. Journal of Chemical Physics, 2000, 112, 220-229.	1.2	140
76	Solvent, isotope, and magnetic field effects in the geminate recombination of radical ion pairs. Journal of Chemical Physics, 1978, 68, 2419-2426.	1.2	138
77	Theoretical Study of the Validity of the Born-Oppenheimer Approximation in the Cl + H2rightarrow HCl + H Reaction. Science, 2002, 296, 715-718.	6.0	138
78	The barrier height of the F+H2 reaction revisited: Coupled-cluster and multireference configuration-interaction benchmark calculations. Journal of Chemical Physics, 2008, 128, 034305.	1.2	136
79	Dissociation of NH3 to NH2+H. Journal of Chemical Physics, 1987, 86, 6693-6700.	1.2	134
80	Accurate calculations of intermolecular interaction energies using explicitly correlated wave functions. Physical Chemistry Chemical Physics, 2008, 10, 3400.	1.3	134
81	A short-range gradient-corrected spin density functional in combination with long-range coupled-cluster methods: Application to alkali-metal rare-gas dimers. Chemical Physics, 2006, 329, 276-282.	0.9	133
82	Spinâ€“orbit effects in the reaction of F(2P) with H2. Journal of Chemical Physics, 1998, 109, 5710-5713.	1.2	131
83	The unimolecular dissociation of HCO: I. Oscillations of pure CO stretching resonance widths. Journal of Chemical Physics, 1995, 102, 3593-3611.	1.2	130
84	Explicitly correlated second-order perturbation theory using density fitting and local approximations. Journal of Chemical Physics, 2006, 124, 054114.	1.2	126
85	Scalable Electron Correlation Methods. 3. Efficient and Accurate Parallel Local Coupled Cluster with Pair Natural Orbitals (PNO-LCCSD). Journal of Chemical Theory and Computation, 2017, 13, 3650-3675.	2.3	122
86	The unimolecular dissociation of HCO. II. Comparison of calculated resonance energies and widths with highâ€resolution spectroscopic data. Journal of Chemical Physics, 1996, 105, 4983-5004.	1.2	121
87	Multireference explicitly correlated F12 theories. Molecular Physics, 2013, 111, 607-630.	0.8	121
88	Explicitly correlated local second-order perturbation theory with a frozen geminal correlation factor. Journal of Chemical Physics, 2006, 124, 094103.	1.2	120
89	Scalable Electron Correlation Methods I.: PNO-LMP2 with Linear Scaling in the Molecular Size and Near-Inverse-Linear Scaling in the Number of Processors. Journal of Chemical Theory and Computation, 2015, 11, 484-507.	2.3	118
90	Electron transfer and spin exchange contributing to the magnetic field dependence of the primary photochemical reaction of bacterial photosynthesis. Biochimica Et Biophysica Acta - Bioenergetics, 1978, 502, 255-268.	0.5	116

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91	Theoretical transition probabilities for the OH meinel system. Journal of Molecular Spectroscopy, 1986, 118, 507-529.	0.4	115
92	An explicitly correlated local coupled cluster method for calculations of large molecules close to the basis set limit. Journal of Chemical Physics, 2011, 135, 144117.	1.2	115
93	The dynamics of the reaction OH + D2 â†' HOD + D: Crossed beam experiments and quantum mechanical scattering calculations on ab initio potential energy surfaces. Chemical Physics, 1996, 207, 389-409.	0.9	114
94	Quantum scattering studies of electronically inelastic collisions of CN (Xâ€‰2Î£+,â€‰Aâ€‰2Î) with He. Journal of Chemical Physics, 1989, 91, 5425-5439.	1.2	113
95	Theoretical Aâ€‰1Aâ€˜2â€“Xâ€‰1A1 absorption and emission spectrum of ammonia. Journal of Chemical Physics, 1987, 86, 6677-6692.	1.2	112
96	Classical dynamics for the F + H2 â†' HF + H reaction on a new ab initio potential energy surface. A direct comparison with experiment. Chemical Physics Letters, 1994, 223, 215-226.	1.2	110
97	A comparison of metallophilic attraction in (Xâ€“Mâ€“PH3)2 (Mâ€‰=â€‰Cu, Ag, Au; Xâ€‰=â€‰H, Cl). Physical Chemistry Chemical Physics, 2002, 4, 1006-1013.	1.3	110
98	Eliminating the domain error in local explicitly correlated second-order MÃ¸llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 2008, 129, 101103.	1.2	109
99	Ab Initio Excited-State Dynamics of the Photoactive Yellow Protein Chromophore. Journal of the American Chemical Society, 2003, 125, 12710-12711.	6.6	108
100	Communication: Second-order multireference perturbation theory with explicit correlation: CASPT2-F12. Journal of Chemical Physics, 2010, 133, 141103.	1.2	108
101	Accurateabinitiocalculations of radiative transition probabilities between theAâ€‰3Î£+u,Bâ€‰3Îg,Wâ€‰3Î”u,Bâ€²â€‰3Î£â¯u, andCâ€‰3Îustates of N2. Journal of Chemical Physics, 1984, 81, 2420-2431.	1.2	105
102	Accurate potential energy surface and quantum reaction rate calculations for the H+CH4â†'H2+CH3 reaction. Journal of Chemical Physics, 2006, 124, 164307.	1.2	101
103	The ultraviolet absorption spectrum of the Ã¬Æ’â€‰1Aâ€˜2â†Ì Æ’â€‰1A1 transition of jetâ€cooled ammonia. Journal of Chemical Physics, 1987, 86, 6669-6676.	1.2	98
104	Explicitly correlated multireference configuration interaction with multiple reference functions: Avoided crossings and conical intersections. Journal of Chemical Physics, 2011, 134, 184104.	1.2	98
105	The Extent of Nonâ€“Born-Oppenheimer Coupling in the Reaction of Cl(² P) with para- H ₂. Science, 2008, 322, 573-576.	6.0	95
106	Analytical energy gradients for second-order multireference perturbation theory using density fitting. Journal of Chemical Physics, 2013, 138, 104104.	1.2	93
107	Quantum calculations on the rate constant for the O + OH reaction. Chemical Physics Letters, 1984, 112, 346-350.	1.2	92
108	Comparison of explicitly correlated local coupled-cluster methods with various choices of virtual orbitals. Physical Chemistry Chemical Physics, 2012, 14, 7591.	1.3	91

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109	Scalable Electron Correlation Methods. 4. Parallel Explicitly Correlated Local Coupled Cluster with Pair Natural Orbitals (PNO-LCCSD-F12). Journal of Chemical Theory and Computation, 2017, 13, 4871-4896.	2.3	91
110	The F+HDâ†'DF(HF)+H(D) reaction revisited: Quasiclassical trajectory study on anabinitiopotential energy surface and comparison with molecular beam experiments. Journal of Chemical Physics, 1995, 102, 9248-9262.	1.2	90
111	The CIPT2 method: Coupling of multi-reference configuration interaction and multi-reference perturbation theory. Application to the chromium dimer. Molecular Physics, 2004, 102, 2369-2379.	0.8	85
112	Accurate multireference configuration interaction calculations of the potential energy function and the dissociation energy of N2. Journal of Chemical Physics, 1991, 94, 1264-1270.	1.2	83
113	Local correlation methods with a natural localized molecular orbital basis. Molecular Physics, 2007, 105, 2753-2761.	0.8	83
114	Calculation of smooth potential energy surfaces using local electron correlation methods. Journal of Chemical Physics, 2006, 125, 184110.	1.2	82
115	Spin-orbit interaction in heavy group 13 atoms and TlAr. Chemical Physics, 1997, 217, 19-27.	0.9	81
116	Quantum mechanical and quasiclassical simulations of molecular beam experiments for the F+H2â†'HF+H reaction on two ab initio potential energy surfaces. Journal of Chemical Physics, 1998, 109, 7224-7237.	1.2	81
117	Accurate calculation of anharmonic vibrational frequencies of medium sized molecules using local coupled cluster methods. Journal of Chemical Physics, 2007, 126, 134108.	1.2	81
118	The orbital-specific virtual local triples correction: OSV-L(T). Journal of Chemical Physics, 2013, 138, 054109.	1.2	81
119	Scalable Electron Correlation Methods. 5. Parallel Perturbative Triples Correction for Explicitly Correlated Local Coupled Cluster with Pair Natural Orbitals. Journal of Chemical Theory and Computation, 2018, 14, 198-215.	2.3	81
120	Chapter 4 On the Selection of Domains and Orbital Pairs in Local Correlation Treatments. Annual Reports in Computational Chemistry, 2006, 2, 53-80.	0.9	80
121	Calculation of the electronic spectrum for Arâ€"OH. Journal of Chemical Physics, 1990, 93, 3367-3378.	1.2	79
122	Toward accurate barriers for enzymatic reactions: QM/MM case study on p-hydroxybenzoate hydroxylase. Journal of Chemical Physics, 2008, 128, 025104.	1.2	79
123	Explicitly correlated composite thermochemistry of transition metal species. Journal of Chemical Physics, 2013, 139, 094302.	1.2	79
124	Local complete active space second-order perturbation theory using pair natural orbitals (PNO-CASPT2). Journal of Chemical Physics, 2016, 145, 124115.	1.2	79
125	Energetics and spinâ€•and Î›â€doublet selectivity in the infrared multiphoton dissociation HN3(X̃ƒâ€‰1Aâ€™)â†'N2(Xâ€‰1Σ+g)+NH(X3Σâˆ',aâ€‰1Δ"): Theory. Journal of Chemical Physics, 1988, 89, 1388-1400.	1.2	78
126	Theoretical spinâ€"rovibronic 2A1(Îu)â€"2B1 spectrum of the H2O+, HDO+, and D2O+ cations. Journal of Chemical Physics, 1993, 98, 5222-5234.	1.2	77

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127	Time-dependent quantum simulations of FH2â^' photoelectron spectra on new ab initio potential energy surfaces for the anionic and the neutral species. Chemical Physics Letters, 1997, 280, 430-438.	1.2	77
128	Integral transformation with low-order scaling for large local second-order Mï¿½ller-Plesset calculations. Journal of Computational Chemistry, 1998, 19, 1241-1254.	1.5	76
129	Ab initio study of the O2 binding in dicopper complexes. Theoretical Chemistry Accounts, 2005, 114, 309-317.	0.5	76
130	Correlation regions within a localized molecular orbital approach. Journal of Chemical Physics, 2008, 128, 144106.	1.2	76
131	Abinitioinvestigation of the bound rovibrational states in the electronic ground state of HeN+2. Journal of Chemical Physics, 1988, 89, 2178-2184.	1.2	75
132	Integral-direct electron correlation methods. Molecular Physics, 1999, 96, 719-733.	0.8	75
133	Experimental and Theoretical Studies of the d8â^'d10Interaction between Pd(II) and Au(I):Â Bis(chloro[(phenylthiomethyl)diphenylphosphine]gold(I))â^'dichloropalladium(II) and Related Systems. Inorganic Chemistry, 2000, 39, 4786-4792.	1.9	75
134	Impact of Local and Density Fitting Approximations on Harmonic Vibrational Frequencies. Journal of Physical Chemistry A, 2006, 110, 2060-2064.	1.1	75
135	Quantum-mechanical calculation of the thermal rate constant for the H2+Clâ†'H+HCl reaction. Chemical Physics Letters, 1999, 313, 647-654.	1.2	74
136	Impact of local approximations on MP2 vibrational frequencies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1999, 55, 647-658.	2.0	72
137	Analytical energy gradients for local coupled-cluster methodsElectronic Supplementary Information available. See http://www.rsc.org/suppdata/cp/b1/b105126c/. Physical Chemistry Chemical Physics, 2001, 3, 4853-4862.	1.3	72
138	Ab initio calculations of radiative transition probabilities in SH, SH+, and SHâ^'. Journal of Chemical Physics, 1985, 83, 4661-4667.	1.2	71
139	The Electronic Ground State of [Fe(CO)₃(NO)]^{â^'}: A Spectroscopic and Theoretical Study. Angewandte Chemie - International Edition, 2014, 53, 1790-1794.	7.2	71
140	Communication: Improved pair approximations in local coupled-cluster methods. Journal of Chemical Physics, 2015, 142, 121102.	1.2	71
141	A theoretical rotationally resolved infrared spectrum for H2O+ (Xâ€‰2B1). Journal of Chemical Physics, 1989, 91, 2818-2833.	1.2	70
142	Bent valence excited states of CO2. Journal of Chemical Physics, 1992, 97, 8382-8388.	1.2	69
143	Ab initiorelativistic pseudopotential study of small silver and gold sulfide clusters (M2S)n, n=1 and 2. Journal of Chemical Physics, 1998, 109, 3096-3107.	1.2	68
144	NMR chemical shift calculations within local correlation methods: the GIAO-LMP2 approach. Physical Chemistry Chemical Physics, 2000, 2, 2083-2090.	1.3	68

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145	Second-order MCSCF optimization revisited. I. Improved algorithms for fast and robust second-order CASSCF convergence. Journal of Chemical Physics, 2019, 150, 194106.	1.2	68
146	Ab initio calculations of coupled potential energy surfaces for the Cl(2P3/2,2P1/2)+ H2 reaction. Physical Chemistry Chemical Physics, 2004, 6, 4975.	1.3	67
147	Scalable Electron Correlation Methods. 2. Parallel PNO-LMP2-F12 with Near Linear Scaling in the Molecular Size. Journal of Chemical Theory and Computation, 2015, 11, 5291-5304.	2.3	67
148	Theoretical rotationalâ€“vibrational spectrum of H2S. Journal of Chemical Physics, 1989, 90, 783-794.	1.2	65
149	A full-CI study of the energetics of the reaction F + H2 â†' HF+H. Chemical Physics Letters, 1991, 185, 555-561.	1.2	65
150	The photodissociation of ClO2: Potential energy surfaces of OClOâ†'Cl+O2. Journal of Chemical Physics, 1996, 105, 9823-9832.	1.2	65
151	The effect of local approximations in coupled-cluster wave functions on dipole moments and static dipole polarisabilities. Physical Chemistry Chemical Physics, 2004, 6, 2059-2065.	1.3	64
152	Benchmark Studies for Explicitly Correlated Perturbation- and Coupled Cluster Theories. javascript:filterformular(Â´3Â´). Zeitschrift Fur Physikalische Chemie, 2010, 224, 493-511.	1.4	64
153	Efficient Explicitly Correlated Coupled-Cluster Approximations. Challenges and Advances in Computational Chemistry and Physics, 2010, , 573-619.	0.6	62
154	MCSCF calculation of the dipole moment function of CO. Molecular Physics, 1981, 44, 111-123.	0.8	59
155	Ab InitioSimulation of Molecular Beam Experiments for the F + H2â†' HF + H Reaction. Journal of Physical Chemistry A, 1997, 101, 6403-6414.	1.1	59
156	New ab initio potential energy surfaces for the F+H2 reaction. Journal of Chemical Physics, 2007, 127, 174302.	1.2	59
157	Vibrational relaxation of N2 by collision with He atoms. Journal of Chemical Physics, 1986, 84, 3788-3797.	1.2	56
158	Unimolecular dissociation dynamics of highly vibrationally excited DCO(XÌƒâ€‰2A). II. Calculation of resonance energies and widths and comparison with high-resolution spectroscopic data. Journal of Chemical Physics, 1997, 106, 5359-5378.	1.2	56
159	Experimental and theoretical differential cross sections for the reactions Cl+H2/D2. Journal of Chemical Physics, 2001, 114, 10662-10672.	1.2	56
160	Theoretical investigation of collision induced rotational alignment in N+2â€“He. Journal of Chemical Physics, 1990, 93, 4687-4698.	1.2	55
161	Accurate thermochemistry from explicitly correlated distinguishable cluster approximation. Journal of Chemical Physics, 2015, 142, 064111.	1.2	55
162	Differential Cross Sections from Quantum Calculations on CoupledAb InitioPotential Energy Surfaces and Scattering Experiments forCl(P2)+H2Reactions. Physical Review Letters, 2003, 91, 013201.	2.9	54

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163	PNOâ€CEPA and MCSCFâ€SCEP calculations of transition probabilities in OH, HF+, and HCl+. Journal of Chemical Physics, 1984, 80, 831-839.	1.2	53
164	Multireferenceâ€CI calculations of radiative transition probabilities in Câ‚‚. Journal of Chemical Physics, 1984, 80, 5085-5088.	1.2	52
165	A joint experimental and theoretical study of Aâ€‰2Îâ†'Xâ€‰2Î£+ electronic energy transfer in the CN molecule induced by collisions with helium. Journal of Chemical Physics, 1993, 98, 8580-8592.	1.2	52
166	Role of Tunneling in the Enzyme Glutamate Mutase. Journal of Physical Chemistry B, 2012, 116, 13682-13689.	1.2	52
167	Multireference CI calculations of radiative transition probabilities between low lying quartet states of the C2+ ion. Journal of Electron Spectroscopy and Related Phenomena, 1986, 41, 289-296.	0.8	51
168	Improved intermolecular water potential from global geometry optimization of small water clusters using local MP2. Chemical Physics, 1998, 239, 561-572.	0.9	51
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