Hans-Joachim Werner

List of Publications by Year
in descending order

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310 papers	53,429 citations	1980 101 h-index	1250 226 g-index
322 all docs	322 docs citations	322 times ranked	11459 citing authors

#	Article	IF	Citations
1	Scalable Electron Correlation Methods. 8. Explicitly Correlated Open-Shell Coupled-Cluster with Pair Natural Orbitals PNO-RCCSD(T)-F12 and PNO-UCCSD(T)-F12. Journal of Chemical Theory and Computation, 2021, 17, 902-926.	2.3	26
2	MCSCF optimization revisited. II. Combined first- and second-order orbital optimization for large molecules. Journal of Chemical Physics, 2020, 152, 074102.	1.2	38
3	Atoms and molecules in soft confinement potentials. Molecular Physics, 2020, 118, e1730989.	0.8	18
4	Breaking established paradigms: a tribute to Wilfried Meyer's contributions to ab initio quantum chemistry. Molecular Physics, 2020, 118, e1730993.	0.8	0
5	Scalable Electron Correlation Methods. 7. Local Open-Shell Coupled-Cluster Methods Using Pair Natural Orbitals: PNO-RCCSD and PNO-UCCSD. Journal of Chemical Theory and Computation, 2020, 16, 3135-3151.	2.3	22
6	The Molpro quantum chemistry package. Journal of Chemical Physics, 2020, 152, 144107.	1.2	603
7	Correspondence on â€œCore Electron Topologies in Chemical Compounds: Case Study of Carbon versus Siliconâ€• Angewandte Chemie, 2019, 131, 10512-10515.	1.6	3
8	Correspondence on â€œCore Electron Topologies in Chemical Compounds: Case Study of Carbon versus Siliconâ€• Angewandte Chemie - International Edition, 2019, 58, 10404-10407.	7.2	2
9	Multi-state local complete active space second-order perturbation theory using pair natural orbitals (PNO-MS-CASPT2). Journal of Chemical Physics, 2019, 150, 214107.	1.2	17
10	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
11	Toward fast and accurate ab initio calculation of magnetic exchange in polynuclear lanthanide complexes. Physical Chemistry Chemical Physics, 2019, 21, 9769-9778.	1.3	12
12	Perturbation Expansion of Internally Contracted Coupled-Cluster Theory up to Third Order. Journal of Chemical Theory and Computation, 2019, 15, 2291-2305.	2.3	14
13	Scalable Electron Correlation Methods. 6. Local Spin-Restricted Open-Shell Second-Order MÃ¸llerâ€“Plesset Perturbation Theory Using Pair Natural Orbitals: PNO-RMP2. Journal of Chemical Theory and Computation, 2019, 15, 987-1005.	2.3	14
14	Accurate Intermolecular Interaction Energies Using Explicitly Correlated Local Coupled Cluster Methods [PNO-LCCSD(T)-F12]. Journal of Chemical Theory and Computation, 2019, 15, 1044-1052.	2.3	35
15	Analytical energy gradients for local second-order MÃ¸ller-Plesset perturbation theory using intrinsic bond orbitals. Molecular Physics, 2019, 117, 1252-1263.	0.8	10
16	Embedded Multireference Coupled Cluster Theory. Journal of Chemical Theory and Computation, 2018, 14, 693-709.	2.3	30
17	Analytical energy gradients for explicitly correlated wave functions. II. Explicitly correlated coupled cluster singles and doubles with perturbative triples corrections: CCSD(T)-F12. Journal of Chemical Physics, 2018, 148, 114104.	1.2	40
18	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

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19	Explicitly correlated local coupledâ€cluster methods using pair natural orbitals. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1371.	6.2	151
20	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
21	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
22	Analytical energy gradients for explicitly correlated wave functions. I. Explicitly correlated second-order MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2017, 147, 214101.	1.2	17
23	Communication: Multipole approximations of distant pair energies in local correlation methods with pair natural orbitals. Journal of Chemical Physics, 2016, 145, 201101.	1.2	39
24	Local complete active space second-order perturbation theory using pair natural orbitals (PNO-CASPT2). Journal of Chemical Physics, 2016, 145, 124115.	1.2	79
25	Parallel and Low-Order Scaling Implementation of Hartreeâ€“Fock Exchange Using Local Density Fitting. Journal of Chemical Theory and Computation, 2016, 12, 3122-3134.	2.3	51
26	Communication: Improved pair approximations in local coupled-cluster methods. Journal of Chemical Physics, 2015, 142, 121102.	1.2	71
27	Accurate thermochemistry from explicitly correlated distinguishable cluster approximation. Journal of Chemical Physics, 2015, 142, 064111.	1.2	55
28	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
29	What Is the Price of Open-Source Software?. Journal of Physical Chemistry Letters, 2015, 6, 2751-2754.	2.1	19
30	On the use of Abelian point group symmetry in density-fitted local MP2 using various types of virtual orbitals. Journal of Chemical Physics, 2015, 142, 164108.	1.2	14
31	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
32	Synthesis and characterization of fluorinated and sulfonated poly(arylene ether-1,3,4-oxadiazole) derivatives and their blend membranes. European Polymer Journal, 2014, 52, 76-87.	2.6	15
33	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
34	Multireference explicitly correlated F12 theories. Molecular Physics, 2013, 111, 607-630.	0.8	121
35	Explicitly correlated composite thermochemistry of transition metal species. Journal of Chemical Physics, 2013, 139, 094302.	1.2	79
36	Pyrazine excited states revisited using the extended multi-state complete active space second-order perturbation method. Physical Chemistry Chemical Physics, 2013, 15, 262-269.	1.3	36

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37	Analytical energy gradients for second-order multireference perturbation theory using density fitting. Journal of Chemical Physics, 2013, 138, 104104.	1.2	93
38	The orbital-specific virtual local triples correction: OSV-L(T). Journal of Chemical Physics, 2013, 138, 054109.	1.2	81
39	The orbital-specific-virtual local coupled cluster singles and doubles method. Journal of Chemical Physics, 2012, 136, 144105.	1.2	163
40	Comparison of explicitly correlated local coupled-cluster methods with various choices of virtual orbitals. Physical Chemistry Chemical Physics, 2012, 14, 7591.	1.3	91
41	Role of Tunneling in the Enzyme Glutamate Mutase. Journal of Physical Chemistry B, 2012, 116, 13682-13689.	1.2	52
42	Molpro: a generalâ€purpose quantum chemistry program package. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 242-253.	6.2	2,852
43	Determining the Numerical Stability of Quantum Chemistry Algorithms. Journal of Chemical Theory and Computation, 2011, 7, 2387-2398.	2.3	25
44	An efficient local coupled cluster method for accurate thermochemistry of large systems. Journal of Chemical Physics, 2011, 135, 144116.	1.2	244
45	Explicitly correlated multireference configuration interaction: MRCI-F12. Journal of Chemical Physics, 2011, 134, 034113.	1.2	223
46	Explicitly correlated multireference configuration interaction with multiple reference functions: Avoided crossings and conical intersections. Journal of Chemical Physics, 2011, 134, 184104.	1.2	98
47	A new internally contracted multi-reference configuration interaction method. Journal of Chemical Physics, 2011, 135, 054101.	1.2	246
48	Explicitly correlated coupled cluster methods with pair-specific geminals. Molecular Physics, 2011, 109, 407-417.	0.8	200
49	Communication: Non-adiabatic coupling and resonances in the F + H2 reaction at low energies. Journal of Chemical Physics, 2011, 134, 231101.	1.2	45
50	A combined quantum mechanical and experimental approach towards chiral diketopiperazine hydroperoxides. Journal of Physical Organic Chemistry, 2011, 24, 682-692.	0.9	6
51	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
52	Application of explicitly correlated coupled-cluster methods to molecules containing post-3d main group elements. Molecular Physics, 2011, 109, 2607-2623.	0.8	33
53	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
54	Local Approximations for an Efficient and Accurate Treatment of Electron Correlation and Electron Excitations in Molecules. Challenges and Advances in Computational Chemistry and Physics, 2011, , 345-407.	0.6	27

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55	Coupling of Short-range Density-functional with Long-range Post-Hartree-Fock Methods. Zeitschrift Fur Physikalische Chemie, 2010, 224, 481-491.	1.4	2
56	Efficient Explicitly Correlated Coupled-Cluster Approximations. Challenges and Advances in Computational Chemistry and Physics, 2010, , 573-619.	0.6	62
57	Reductive half-reaction of aldehyde oxidoreductase toward acetaldehyde: Ab initio and free energy quantum mechanical/molecular mechanical calculations. Journal of Chemical Physics, 2010, 132, 035101.	1.2	33
58	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
59	Communication: Second-order multireference perturbation theory with explicit correlation: CASPT2-F12. Journal of Chemical Physics, 2010, 133, 141103.	1.2	108
60	Analytic gradients for the combinedsr-DFT/lr-MP2 method: application to weakly bound systems. Molecular Physics, 2010, 108, 3373-3382.	0.8	8
61	Coupling of Short-range Density-functional with Long-range Post-Hartree-Fock Methods. , 2010, , 191-201.		0
62	Benchmark Studies for Explicitly Correlated Perturbation- and Coupled Cluster Theories. , 2010, , 203-221.		0
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	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
65	Accurate calculation of vibrational frequencies using explicitly correlated coupled-cluster theory. Journal of Chemical Physics, 2009, 130, 054105.	1.2	173
66	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
67	Simplified CCSD(T)-F12 methods: Theory and benchmarks. Journal of Chemical Physics, 2009, 130, 054104.	1.2	1,558
68	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
69	High-level Ab-initio Calculations for Astrochemically Relevant Polyynes (HC_{2n}H), their Isomers (C_{2n}H₂) and their Anions (C_{2n}H^{â^'}). Zeitschrift Fur Physikalische Chemie, 2009, 223, 447-460.	1.4	6
70	Short-range density functionals in combination with local long-range ab initio methods: Application to non-bonded complexes. Chemical Physics, 2008, 346, 257-265.	0.9	32
71	Explicitly correlated RMP2 for high-spin open-shell reference states. Journal of Chemical Physics, 2008, 128, 154103.	1.2	242
72	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

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73	Toward accurate barriers for enzymatic reactions: QM/MM case study on p-hydroxybenzoate hydroxylase. Journal of Chemical Physics, 2008, 128, 025104.	1.2	79
74	Accurate calculations of intermolecular interaction energies using explicitly correlated wave functions. Physical Chemistry Chemical Physics, 2008, 10, 3400.	1.3	134
75	Local and density fitting approximations within the short-range/long-range hybrid scheme: application to large non-bonded complexes. Physical Chemistry Chemical Physics, 2008, 10, 3353.	1.3	48
76	The accuracy of local MP2 methods for conformational energies. Molecular Physics, 2008, 106, 1899-1906.	0.8	29
77	Correlation regions within a localized molecular orbital approach. Journal of Chemical Physics, 2008, 128, 144106.	1.2	76
78	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
79	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
80	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
81	Evidence for excited spin-orbit state reaction dynamics in F+H2: Theory and experiment. Journal of Chemical Physics, 2008, 128, 084313.	1.2	31
82	Matrix-Formulated Direct Multiconfiguration Self-Consistent Field and Multiconfiguration Reference Configuration-Interaction Methods. Advances in Chemical Physics, 2007, , 1-62.	0.3	205
83	Ab initio potential energy surface and spectrum of the B(Î3) state of the HeI2 complex. Journal of Chemical Physics, 2007, 126, 204301.	1.2	31
84	Comparing electronic structure predictions for the ground state dissociation of vinoxy radicals. Journal of Chemical Physics, 2007, 127, 094309.	1.2	7
85	General orbital invariant MP2-F12 theory. Journal of Chemical Physics, 2007, 126, 164102.	1.2	490
86	New ab initio potential energy surfaces for the F+H2 reaction. Journal of Chemical Physics, 2007, 127, 174302.	1.2	59
87	Local correlation methods with a natural localized molecular orbital basis. Molecular Physics, 2007, 105, 2753-2761.	0.8	83
88	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
89	High-Accuracy Extrapolated Ab Initio Thermochemistry of Vinyl Chloride. Journal of Physical Chemistry A, 2007, 111, 13623-13628.	1.1	13
90	Calculation of transition moments between internally contracted MRCI wave functions with non-orthogonal orbitalsâ€. Molecular Physics, 2007, 105, 1239-1249.	0.8	22

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91	Breakdown of the Born-Oppenheimer Approximation in the F+ o -D ₂ â†' DF + D Reaction. Science, 2007, 317, 1061-1064.	6.0	149
92	A simple and efficient CCSD(T)-F12 approximation. Journal of Chemical Physics, 2007, 127, 221106.	1.2	1,587
93	Explicitly correlated second-order perturbation theory using density fitting and local approximations. Journal of Chemical Physics, 2006, 124, 054114.	1.2	126
94	Impact of Local and Density Fitting Approximations on Harmonic Vibrational Frequencies. Journal of Physical Chemistry A, 2006, 110, 2060-2064.	1.1	75
95	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
96	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
97	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
98	High-Accuracy Computation of Reaction Barriers in Enzymes. Angewandte Chemie - International Edition, 2006, 45, 6856-6859.	7.2	253
99	Explicitly correlated local second-order perturbation theory with a frozen geminal correlation factor. Journal of Chemical Physics, 2006, 124, 094103.	1.2	120
100	Calculation of smooth potential energy surfaces using local electron correlation methods. Journal of Chemical Physics, 2006, 125, 184110.	1.2	82
101	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
102	Application of Gaussian-type geminals in local second-order MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2006, 124, 234107.	1.2	25
103	Comparative calculations for the A-frame molecules [S(MPH3)2] (M=Cu, Ag, Au) at levels up to CCSD(T). Chemical Physics Letters, 2005, 405, 148-152.	1.2	38
104	Towards Accurate ab initio Calculations on the Vibrational Modes of the Alkaline Earth Metal Hydrides.. ChemInform, 2005, 36, no.	0.1	0
105	Ab initio study of the O2 binding in dicopper complexes. Theoretical Chemistry Accounts, 2005, 114, 309-317.	0.5	76
106	Effect of rotational energy on the reaction Li+HF(Ï...=0,j)â†'LiF+H: An experimental and computational study. Journal of Chemical Physics, 2005, 122, 244304.	1.2	28
107	Towards accurate ab initio calculations on the vibrational modes of the alkaline earth metal hydrides. Physical Chemistry Chemical Physics, 2005, 7, 3123.	1.3	40
108	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

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109	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
110	A theoretical study of the electronically excited states in linear and cyclic. Molecular Physics, 2004, 102, 2227-2236.	0.8	9
111	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
112	First-Principles Theory for the H + CH4 -> H2 + CH3 Reaction. Science, 2004, 306, 2227-2229.	6.0	238
113	Fast Hartreeâ€"Fock theory using local density fitting approximations. Molecular Physics, 2004, 102, 2311-2321.	0.8	276
114	Wave packet calculations for the Cl + H2reaction. International Journal of Quantum Chemistry, 2004, 96, 562-567.	1.0	29
115	Rotational and alignment effects in a wave packet calculation for the Cl + H2reaction. International Journal of Quantum Chemistry, 2004, 99, 577-584.	1.0	18
116	Details and consequences of the nonadiabatic coupling in the Cl(2P)â€‰+â€‰H2reaction. Faraday Discussions, 2004, 127, 59-72.	1.6	48
117	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
118	Rotational and alignment effects in a multisurface wavepacket calculation for the Cl + H2reaction. Physical Chemistry Chemical Physics, 2004, 6, 5000-5006.	1.3	13
119	The effect of spinâ€"orbit coupling on the thermal rate constant of the H2+ Cl â†' H + HCl reaction. Physical Chemistry Chemical Physics, 2004, 6, 5026-5030.	1.3	26
120	The dynamics of the prototype abstraction reaction Cl(2P3/2,1/2)+ H2: A comparison of crossed molecular beam experiments with exact quantum scattering calculations on coupled ab initio potential energy surfaces. Physical Chemistry Chemical Physics, 2004, 6, 5007.	1.3	36
121	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
122	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
123	The vibrational spectra of furoxan and dichlorofuroxan: A comparative theoretical study using density functional theory and local electron correlation methods. Physical Chemistry Chemical Physics, 2003, 5, 2001.	1.3	32
124	Exchange-correlation energies and correlation holes for some two- and four-electron atoms along a nonlinear adiabatic connection in density functional theory. International Journal of Quantum Chemistry, 2003, 91, 84-93.	1.0	36
125	Ab Initio Excited-State Dynamics of the Photoactive Yellow Protein Chromophore. Journal of the American Chemical Society, 2003, 125, 12710-12711.	6.6	108
126	Analytical energy gradients for internally contracted second-order multireference perturbation theory. Journal of Chemical Physics, 2003, 119, 5044-5057.	1.2	248

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127	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
128	Local treatment of electron excitations in the EOM-CCSD method. Journal of Chemical Physics, 2003, 118, 3006-3019.	1.2	273
129	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
130	Theoretical Study of the Dissociation and Isomerization of NCS. Zeitschrift Fur Physikalische Chemie, 2003, 217, 255-264.	1.4	8
131	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
132	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
133	Electron correlation effects on structural and cohesive properties of closo-hydroborate dianions (BnHn)2- (n = 5â€“12) and B4H4. Physical Chemistry Chemical Physics, 2001, 3, 514-522.	1.3	30
134	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
135	Low-order scaling local electron correlation methods. IV. Linear scaling local coupled-cluster (LCCSD). Journal of Chemical Physics, 2001, 114, 661.	1.2	564
136	Calculation of the Raman Spectrum of Photodissociating H2S around 195 nmâ€. Journal of Physical Chemistry A, 2001, 105, 2458-2467.	1.1	7
137	Ab initiocalculations of adiabatic and diabatic potential energy surfaces of Cl(2P)â‹¯HCl(1Î£+) van der Waals complex. Journal of Chemical Physics, 2001, 115, 3085-3098.	1.2	41
138	Experimental and theoretical differential cross sections for the reactions Cl+H2/D2. Journal of Chemical Physics, 2001, 114, 10662-10672.	1.2	56
139	A quantum mechanical and quasi-classical trajectory study of the Cl+H2 reaction and its isotopic variants: Dependence of the integral cross section on the collision energy and reagent rotation. Journal of Chemical Physics, 2001, 115, 2074-2081.	1.2	38
140	The ion-molecule reaction O⁺(⁴S) + N₂(X¹Î£⁺) â†’ NO⁺(X¹Î£⁺,vâ€²) + N(⁴S) and the predissociation of the A²Î£⁺and B²Î states of N₂O⁺. Molecular Physics, 2000, 98, 1793-1802.	0.8	37
141	Local perturbative triples correction (T) with linear cost scaling. Chemical Physics Letters, 2000, 318, 370-378.	1.2	296
142	Dynamics of the Cl+D2 reaction: a comparison of crossed molecular beam experiments with quasi-classical trajectory calculations on a new ab initio potential energy surface. Chemical Physics Letters, 2000, 328, 500-508.	1.2	36
143	Spin-orbit matrix elements for internally contracted multireference configuration interaction wavefunctions. Molecular Physics, 2000, 98, 1823-1833.	0.8	856
144	Perspective on "Theory of self-consistent electron pairs. An iterative method for correlated many-electron wavefunctions". Theoretical Chemistry Accounts, 2000, 103, 322-325.	0.5	2

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145	A fullyab initio potential energy surface for ClH2 reactive system. Science in China Series B: Chemistry, 2000, 43, 396-404.	0.8	1
146	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
147	Multireference perturbation theory for large restricted and selected active space reference wave functions. Journal of Chemical Physics, 2000, 112, 5546-5557.	1.2	791
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149	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
150	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
151	Global ab initio potential energy surfaces for the ClH2 reactive system. Journal of Chemical Physics, 2000, 112, 220-229.	1.2	140
152	Potential energy surfaces for the CN(Xâ€‰2Î£+,Aâ€Š2Î)Ar system and inelastic scattering within the A state. Journal of Chemical Physics, 2000, 112, 781-791.	1.2	48
153	NMR chemical shift calculations within local correlation methods: the GIAO-LMP2 approach. Physical Chemistry Chemical Physics, 2000, 2, 2083-2090.	1.3	68
154	Perspective on â€œTheory of self-consistent electron pairs. An iterative method for correlated many-electron wavefunctionsâ€•, 2000, , 322-325.		0
155	Quartet and sextet states of CSâ^'. Journal of Chemical Physics, 1999, 110, 11835-11840.	1.2	23
156	Integral-direct electron correlation methods. Molecular Physics, 1999, 96, 719-733.	0.8	75
157	Impact of local approximations on MP2 vibrational frequencies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1999, 55, 647-658.	2.0	72
158	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
159	Local interpolation of ab initio potential energy surfaces for direct dynamics studies of chemical reactions. Chemical Physics Letters, 1999, 302, 208-214.	1.2	14
160	The aurophilic attraction as interpreted by local correlation methods. Journal of Chemical Physics, 1999, 110, 7210-7215.	1.2	163
161	van der Waals Interactions in the Cl + HD Reaction. Science, 1999, 286, 1713-1716.	6.0	287
162	Photodissociation dynamics of H2S on new coupled ab initio potential energy surfaces. Journal of Chemical Physics, 1999, 111, 4523-4534.	1.2	159

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163	Low-order scaling local electron correlation methods. I. Linear scaling local MP2. Journal of Chemical Physics, 1999, 111, 5691-5705.	1.2	671
164	Multipole approximation of distant pair energies in local MP2 calculations. Chemical Physics Letters, 1998, 290, 143-149.	1.2	184
165	Integral transformation with low-order scaling for large local second-order Mï¿½ller-Plesset calculations. , 1998, 19, 1241-1254.		76
166	Reaction path following by quadratic steepest descent. Theoretical Chemistry Accounts, 1998, 100, 21-30.	0.5	46
167	Improved intermolecular water potential from global geometry optimization of small water clusters using local MP2. Chemical Physics, 1998, 239, 561-572.	0.9	51
168	Analytical energy gradients for local second-order Mo/llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 1998, 108, 5185-5193.	1.2	204
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