Hans-Joachim Werner

List of Publications by Year in Descending Order

311 papers	47,338 citations	98 h-index	214 g-index
321 ext. papers	50,013 ext. citations	4.2 avg, IF	7.73 L-index

#	Paper	IF	Citations
311	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	6.4	11
310	MCSCF optimization revisited. II. Combined first- and second-order orbital optimization for large molecules. *Journal of Chemical Physics*, **2020**, 152, 074102	3.9	21
309	Atoms and molecules in soft confinement potentials. *Molecular Physics*, **2020**, 118, e1730989	1.7	8
308	Breaking established paradigms: a tribute to Wilfried Meyer's contributions to ab initio quantum chemistry. *Molecular Physics*, **2020**, 118, e1730993	1.7	
307	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	6.4	8
306	The Molpro quantum chemistry package. *Journal of Chemical Physics*, **2020**, 152, 144107	3.9	197
305	Multi-state local complete active space second-order perturbation theory using pair natural orbitals (PNO-MS-CASPT2). *Journal of Chemical Physics*, **2019**, 150, 214107	3.9	10
304	Second-order MCSCF optimization revisited. I. Improved algorithms for fast and robust second-order CASSCF convergence. *Journal of Chemical Physics*, **2019**, 150, 194106	3.9	39
303	Toward fast and accurate ab initio calculation of magnetic exchange in polynuclear lanthanide complexes. *Physical Chemistry Chemical Physics*, **2019**, 21, 9769-9778	3.6	8
302	Perturbation Expansion of Internally Contracted Coupled-Cluster Theory up to Third Order. *Journal of Chemical Theory and Computation*, **2019**, 15, 2291-2305	6.4	11
301	Correspondence on Core Electron Topologies in Chemical Compounds: Case Study of Carbon versus Silicon *Angewandte Chemie*, **2019**, 131, 10512-10515	3.6	1
300	Correspondence on "Core Electron Topologies in Chemical Compounds: Case Study of Carbon versus Silicon". *Angewandte Chemie - International Edition*, **2019**, 58, 10404-10407	16.4	2
299	Scalable Electron Correlation Methods. 6. Local Spin-Restricted Open-Shell Second-Order Møller-Plesset Perturbation Theory Using Pair Natural Orbitals: PNO-RMP2. *Journal of Chemical Theory and Computation*, **2019**, 15, 987-1005	6.4	7
298	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	6.4	24
297	Analytical energy gradients for local second-order Møller-Plesset perturbation theory using intrinsic bond orbitals. *Molecular Physics*, **2019**, 117, 1252-1263	1.7	8
296	Embedded Multireference Coupled Cluster Theory. *Journal of Chemical Theory and Computation*, **2018**, 14, 693-709	6.4	22
295	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	3.9	17

294	Explicitly correlated local coupled-cluster methods using pair natural orbitals. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1371	7.9	94
293	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	6.4	56
292	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	6.4	61
291	Explicitly Correlated Local Electron Correlation Methods **2017**, 1-79		9
290	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	6.4	96
289	Analytical energy gradients for explicitly correlated wave functions. I. Explicitly correlated second-order M□ller-Plesset perturbation theory. *Journal of Chemical Physics*, **2017**, 147, 214101	3.9	11
288	Parallel and Low-Order Scaling Implementation of Hartree-Fock Exchange Using Local Density Fitting. *Journal of Chemical Theory and Computation*, **2016**, 12, 3122-34	6.4	41
287	Communication: Multipole approximations of distant pair energies in local correlation methods with pair natural orbitals. *Journal of Chemical Physics*, **2016**, 145, 201101	3.9	33
286	Local complete active space second-order perturbation theory using pair natural orbitals (PNO-CASPT2). *Journal of Chemical Physics*, **2016**, 145, 124115	3.9	66
285	What Is the Price of Open-Source Software?. *Journal of Physical Chemistry Letters*, **2015**, 6, 2751-4	6.4	8
284	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	3.9	14
283	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, 5291-304	6.4	56
282	Communication: Improved pair approximations in local coupled-cluster methods. *Journal of Chemical Physics*, **2015**, 142, 121102	3.9	63
281	Accurate thermochemistry from explicitly correlated distinguishable cluster approximation. *Journal of Chemical Physics*, **2015**, 142, 064111	3.9	42
280	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	6.4	103
279	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	5.2	14
278	The electronic ground state of [Fe(CO)3 (NO)](-) : a spectroscopic and theoretical study. *Angewandte Chemie - International Edition*, **2014**, 53, 1790-4	16.4	59
277	Der elektronische Grundzustand von [Fe(CO)3(NO)]□eine spektroskopische und theoretische Studie. *Angewandte Chemie*, **2014**, 126, 1820-1824	3.6	32

276	Multireference explicitly correlated F12 theories. *Molecular Physics*, **2013**, 111, 607-630	1.7	92
275	Explicitly correlated composite thermochemistry of transition metal species. *Journal of Chemical Physics*, **2013**, 139, 094302	3.9	69
274	Pyrazine excited states revisited using the extended multi-state complete active space second-order perturbation method. *Physical Chemistry Chemical Physics*, **2013**, 15, 262-9	3.6	30
273	Analytical energy gradients for second-order multireference perturbation theory using density fitting. *Journal of Chemical Physics*, **2013**, 138, 104104	3.9	80
272	The orbital-specific virtual local triples correction: OSV-L(T). *Journal of Chemical Physics*, **2013**, 138, 054109	3.9	69
271	The orbital-specific-virtual local coupled cluster singles and doubles method. *Journal of Chemical Physics*, **2012**, 136, 144105	3.9	142
270	Comparison of explicitly correlated local coupled-cluster methods with various choices of virtual orbitals. *Physical Chemistry Chemical Physics*, **2012**, 14, 7591-604	3.6	82
269	Role of tunneling in the enzyme glutamate mutase. *Journal of Physical Chemistry B*, **2012**, 116, 13682-9	3.4	48
268	Molpro: a general-purpose quantum chemistry program package. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 242-253	7.9	2254
267	An efficient local coupled cluster method for accurate thermochemistry of large systems. *Journal of Chemical Physics*, **2011**, 135, 144116	3.9	226
266	Explicitly correlated multireference configuration interaction: MRCI-F12. *Journal of Chemical Physics*, **2011**, 134, 034113	3.9	189
265	Explicitly correlated multireference configuration interaction with multiple reference functions: avoided crossings and conical intersections. *Journal of Chemical Physics*, **2011**, 134, 184104	3.9	84
264	A new internally contracted multi-reference configuration interaction method. *Journal of Chemical Physics*, **2011**, 135, 054101	3.9	189
263	Explicitly correlated coupled cluster methods with pair-specific geminals. *Molecular Physics*, **2011**, 109, 407-417	1.7	169
262	Communication: non-adiabatic coupling and resonances in the F + H2 reaction at low energies. *Journal of Chemical Physics*, **2011**, 134, 231101	3.9	44
261	A combined quantum mechanical and experimental approach towards chiral diketopiperazine hydroperoxides. *Journal of Physical Organic Chemistry*, **2011**, 24, 682-692	2.1	4
260	Determining the Numerical Stability of Quantum Chemistry Algorithms. *Journal of Chemical Theory and Computation*, **2011**, 7, 2387-98	6.4	22
259	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	3.9	104

258	Application of explicitly correlated coupled-cluster methods to molecules containing post-3d main group elements. *Molecular Physics*, **2011**, 109, 2607-2623	1.7	27
257	Communication: extended multi-state complete active space second-order perturbation theory: energy and nuclear gradients. *Journal of Chemical Physics*, **2011**, 135, 081106	3.9	273
256	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	0.7	26
255	Efficient Explicitly Correlated Coupled-Cluster Approximations. *Challenges and Advances in Computational Chemistry and Physics*, **2010**, 573-619	0.7	54
254	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	3.9	31
253	Benchmark Studies for Explicitly Correlated Perturbation- and Coupled Cluster Theories. javascript:filterformular(□3□). *Zeitschrift Fur Physikalische Chemie*, **2010**, 224, 493-511	3.1	61
252	Communication: Second-order multireference perturbation theory with explicit correlation: CASPT2-F12. *Journal of Chemical Physics*, **2010**, 133, 141103	3.9	98
251	Analytic gradients for the combined sr-DFT/lr-MP2 method: application to weakly bound systems. *Molecular Physics*, **2010**, 108, 3373-3382	1.7	8
250	Coupling of Short-range Density-functional with Long-range Post-Hartree-Fock Methods. *Zeitschrift Fur Physikalische Chemie*, **2010**, 224, 481-491	3.1	2
249	Coupling of Short-range Density-functional with Long-range Post-Hartree-Fock Methods **2010**, 191-201		
248	Benchmark Studies for Explicitly Correlated Perturbation- and Coupled Cluster Theories **2010**, 203-221		
247	Local explicitly correlated second-order perturbation theory for the accurate treatment of large molecules. *Journal of Chemical Physics*, **2009**, 130, 054106	3.9	149
246	Local explicitly correlated coupled-cluster methods: efficient removal of the basis set incompleteness and domain errors. *Journal of Chemical Physics*, **2009**, 130, 241101	3.9	139
245	Accurate calculation of vibrational frequencies using explicitly correlated coupled-cluster theory. *Journal of Chemical Physics*, **2009**, 130, 054105	3.9	154
244	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, 11580-5	2.8	141
243	Simplified CCSD(T)-F12 methods: theory and benchmarks. *Journal of Chemical Physics*, **2009**, 130, 054104	3.9	1272
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241	High-level Ab-initio Calculations for Astrochemically Relevant Polyynes (HC2nH), their Isomers (C2nH2) and their Anions (C2nH□ *Zeitschrift Fur Physikalische Chemie*, **2009**, 223, 447-460	3.1	4

240	Toward accurate barriers for enzymatic reactions: QM/MM case study on p-hydroxybenzoate hydroxylase. *Journal of Chemical Physics*, **2008**, 128, 025104	3.9	75
239	Accurate calculations of intermolecular interaction energies using explicitly correlated wave functions. *Physical Chemistry Chemical Physics*, **2008**, 10, 3400-9	3.6	126
238	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, 3353-7	3.6	45
237	The accuracy of local MP2 methods for conformational energies. *Molecular Physics*, **2008**, 106, 1899-1906	1.7	25
236	Correlation regions within a localized molecular orbital approach. *Journal of Chemical Physics*, **2008**, 128, 144106	3.9	71
235	Eliminating the domain error in local explicitly correlated second-order Møller-Plesset perturbation theory. *Journal of Chemical Physics*, **2008**, 129, 101103	3.9	102
234	The extent of non-Born-Oppenheimer coupling in the reaction of Cl(2P) with para-H2. *Science*, **2008**, 322, 573-6	33.3	88
233	Systematically convergent basis sets for explicitly correlated wavefunctions: the atoms H, He, B-Ne, and Al-Ar. *Journal of Chemical Physics*, **2008**, 128, 084102	3.9	925
232	Evidence for excited spin-orbit state reaction dynamics in F+H2: theory and experiment. *Journal of Chemical Physics*, **2008**, 128, 084313	3.9	30
231	Short-range density functionals in combination with local long-range ab initio methods: Application to non-bonded complexes. *Chemical Physics*, **2008**, 346, 257-265	2.3	31
230	Explicitly correlated RMP2 for high-spin open-shell reference states. *Journal of Chemical Physics*, **2008**, 128, 154103	3.9	220
229	The barrier height of the F+H2 reaction revisited: coupled-cluster and multireference configuration-interaction benchmark calculations. *Journal of Chemical Physics*, **2008**, 128, 034305	3.9	122
228	Accurate calculation of anharmonic vibrational frequencies of medium sized molecules using local coupled cluster methods. *Journal of Chemical Physics*, **2007**, 126, 134108	3.9	75
227	High-accuracy extrapolated ab initio thermochemistry of vinyl chloride. *Journal of Physical Chemistry A*, **2007**, 111, 13623-8	2.8	13
226	Calculation of transition moments between internally contracted MRCI wave functions with non-orthogonal orbitals. View all notes. *Molecular Physics*, **2007**, 105, 1239-1249	1.7	21
225	Breakdown of the Born-Oppenheimer approximation in the F+ o-D2 -> DF + D reaction. *Science*, **2007**, 317, 1061-4	33.3	141
224	A simple and efficient CCSD(T)-F12 approximation. *Journal of Chemical Physics*, **2007**, 127, 221106	3.9	1318
223	Matrix-Formulated Direct Multiconfiguration Self-Consistent Field and Multiconfiguration Reference Configuration-Interaction Methods. *Advances in Chemical Physics*, **2007**, 1-62		171

222	Ab initio potential energy surface and spectrum of the B(3Pi) state of the HeI2 complex. *Journal of Chemical Physics*, **2007**, 126, 204301	3.9	30
221	Comparing electronic structure predictions for the ground state dissociation of vinoxy radicals. *Journal of Chemical Physics*, **2007**, 127, 094309	3.9	7
220	General orbital invariant MP2-F12 theory. *Journal of Chemical Physics*, **2007**, 126, 164102	3.9	436
219	New ab initio potential energy surfaces for the F+ H2 reaction. *Journal of Chemical Physics*, **2007**, 127, 174302	3.9	56
218	Local correlation methods with a natural localized molecular orbital basis. *Molecular Physics*, **2007**, 105, 2753-2761	1.7	75
217	High-accuracy computation of reaction barriers in enzymes. *Angewandte Chemie - International Edition*, **2006**, 45, 6856-9	16.4	223
216	High-Accuracy Computation of Reaction Barriers in Enzymes. *Angewandte Chemie*, **2006**, 118, 7010-7013	3.6	56
215	Explicitly correlated local second-order perturbation theory with a frozen geminal correlation factor. *Journal of Chemical Physics*, **2006**, 124, 94103	3.9	118
214	Calculation of smooth potential energy surfaces using local electron correlation methods. *Journal of Chemical Physics*, **2006**, 125, 184110	3.9	80
213	Chapter 4 On the Selection of Domains and Orbital Pairs in Local Correlation Treatments. *Annual Reports in Computational Chemistry*, **2006**, 2, 53-80	1.8	78
212	Application of Gaussian-type geminals in local second-order M□ller-Plesset perturbation theory. *Journal of Chemical Physics*, **2006**, 124, 234107	3.9	25
211	Explicitly correlated second-order perturbation theory using density fitting and local approximations. *Journal of Chemical Physics*, **2006**, 124, 054114	3.9	124
210	Impact of local and density fitting approximations on harmonic vibrational frequencies. *Journal of Physical Chemistry A*, **2006**, 110, 2060-4	2.8	75
209	Accurate potential energy surface and quantum reaction rate calculations for the H+CH4-->H2+CH3 reaction. *Journal of Chemical Physics*, **2006**, 124, 164307	3.9	95
208	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	2.3	125
207	Calculation of intermolecular interactions in the benzene dimer using coupled-cluster and local electron correlation methods. *Physical Chemistry Chemical Physics*, **2006**, 8, 4072-8	3.6	206
206	Towards accurate ab initio calculations on the vibrational modes of the alkaline earth metal hydrides. *Physical Chemistry Chemical Physics*, **2005**, 7, 3123-5	3.6	34
205	A short-range gradient-corrected density functional in long-range coupled-cluster calculations for rare gas dimers. *Physical Chemistry Chemical Physics*, **2005**, 7, 3917-23	3.6	180

204	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	2.5	36
203	Ab initio study of the O2 binding in dicopper complexes. *Theoretical Chemistry Accounts*, **2005**, 114, 309-317	1.9	70
202	Effect of rotational energy on the reaction Li + HF(upsilon = 0,j)-->LiF + H: an experimental and computational study. *Journal of Chemical Physics*, **2005**, 122, 244304	3.9	25
201	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	1.7	79
200	A theoretical study of the electronically excited states in linear and cyclic. *Molecular Physics*, **2004**, 102, 2227-2236	1.7	7
199	Dynamically weighted multiconfiguration self-consistent field: multistate calculations for F+H2O-->HF+OH reaction paths. *Journal of Chemical Physics*, **2004**, 120, 7281-9	3.9	137
198	First-principles theory for the H + CH4 --> H2 + CH3 reaction. *Science*, **2004**, 306, 2227-9	33.3	227
197	Fast Hartree–Fock theory using local density fitting approximations. *Molecular Physics*, **2004**, 102, 2311-2321	1.7	257
196	Wave packet calculations for the Cl + H2 reaction. *International Journal of Quantum Chemistry*, **2004**, 96, 562-567	2.1	26
195	Rotational and alignment effects in a wave packet calculation for the Cl + H2 reaction. *International Journal of Quantum Chemistry*, **2004**, 99, 577-584	2.1	17
194	Details and consequences of the nonadiabatic coupling in the Cl(2P) + H2 reaction. *Faraday Discussions*, **2004**, 127, 59-72	3.6	43
193	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	3.6	62
192	Rotational and alignment effects in a multisurface wavepacket calculation for the Cl + H2 reaction. *Physical Chemistry Chemical Physics*, **2004**, 6, 5000-5006	3.6	13
191	The effect of spin–orbit coupling on the thermal rate constant of the H2 + Cl -> H + HCl reaction. *Physical Chemistry Chemical Physics*, **2004**, 6, 5026-5030	3.6	24
190	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	3.6	36
189	Ab initio calculations of coupled potential energy surfaces for the Cl(2P3/2,2P1/2) + H2 reaction. *Physical Chemistry Chemical Physics*, **2004**, 6, 4975	3.6	66
188	Analytical energy gradients for local second-order Möller-Plesset perturbation theory using density fitting approximations. *Journal of Chemical Physics*, **2004**, 121, 737-50	3.9	206
187	Fast linear scaling second-order Möller-Plesset perturbation theory (MP2) using local and density fitting approximations. *Journal of Chemical Physics*, **2003**, 118, 8149-8160	3.9	606

186	Theoretical Study of the Dissociation and Isomerization of NCS. *Zeitschrift Fur Physikalische Chemie*, **2003**, 217, 255-264	3.1	8
185	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	3.6	31
184	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	2.1	34
183	Ab initio excited-state dynamics of the photoactive yellow protein chromophore. *Journal of the American Chemical Society*, **2003**, 125, 12710-1	16.4	103
182	Analytical energy gradients for internally contracted second-order multireference perturbation theory. *Journal of Chemical Physics*, **2003**, 119, 5044-5057	3.9	229
181	Differential cross sections from quantum calculations on coupled Ab initio potential energy surfaces and scattering experiments for Cl(2P)+H2 reactions. *Physical Review Letters*, **2003**, 91, 013201	7.4	54
180	Local treatment of electron excitations in the EOM-CCSD method. *Journal of Chemical Physics*, **2003** , 118, 3006-3019	3.9	241
179	Theoretical study of the validity of the Born-Oppenheimer approximation in the Cl + H2 --> HCl + H reaction. *Science*, **2002**, 296, 715-8	33.3	128
178	A comparison of metallophilic attraction in (XMPH3)2(M = Cu, Ag, Au; X = H, Cl). *Physical Chemistry Chemical Physics*, **2002**, 4, 1006-1013	3.6	102
177	Ab initio calculations of adiabatic and diabatic potential energy surfaces of Cl(2P)?HCl(1) van der Waals complex. *Journal of Chemical Physics*, **2001**, 115, 3085-3098	3.9	41
176	Experimental and theoretical differential cross sections for the reactions Cl+H2/D2. *Journal of Chemical Physics*, **2001**, 114, 10662-10672	3.9	52
175	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	3.9	33
174	Electron correlation effects on structural and cohesive properties of closo-hydroborate dianions (BnHn)2(n= 512) and B4H4. *Physical Chemistry Chemical Physics*, **2001**, 3, 514-522	3.6	27
173	Analytical energy gradients for local coupled-cluster methods. *Physical Chemistry Chemical Physics*, **2001**, 3, 4853-4862	3.6	70
172	Low-order scaling local electron correlation methods. IV. Linear scaling local coupled-cluster (LCCSD). *Journal of Chemical Physics*, **2001**, 114, 661	3.9	521
171	Calculation of the Raman Spectrum of Photodissociating H2S around 195 nm *Journal of Physical Chemistry A*, **2001**, 105, 2458-2467	2.8	6
170	The ion-molecule reaction O+ (4S) + N2(X1) -> NO+ (X1+, v?) + N(4S) and the predissociation of the A2 and B2states of N2O+. *Molecular Physics*, **2000**, 98, 1793-1802	1.7	31
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168	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	2.5	31
167	Spin-orbit matrix elements for internally contracted multireference configuration interaction wavefunctions. *Molecular Physics*, **2000**, 98, 1823-1833	1.7	741
166	Perspective on Theory of self-consistent electron pairs. An iterative method for correlated many-electron wavefunctions *Theoretical Chemistry Accounts*, **2000**, 103, 322-325	1.9	2
165	A fullyab initio potential energy surface for ClH2 reactive system. *Science in China Series B: Chemistry*, **2000**, 43, 396-404		1
164	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	3.9	224
163	Multireference perturbation theory for large restricted and selected active space reference wave functions. *Journal of Chemical Physics*, **2000**, 112, 5546-5557	3.9	690
162	Convergence of Breit Pauli spin orbit matrix elements with basis set size and configuration interaction space: The halogen atoms F, Cl, and Br. *Journal of Chemical Physics*, **2000**, 112, 5624-5632	3.9	43
161	Low-order scaling local correlation methods II: Splitting the Coulomb operator in linear scaling local second-order M ller Plesset perturbation theory. *Journal of Chemical Physics*, **2000**, 113, 9443-9455	3.9	189
160	Experimental and theoretical studies of the d8-d10 interaction between Pd(II) and Au(I): bis(chloro[(phenylthiomethyl)diphenylphosphine]gold(I))- dichloropalladium(II) and related systems. *Inorganic Chemistry*, **2000**, 39, 4786-92	5.1	65
159	Global ab initio potential energy surfaces for the ClH2 reactive system. *Journal of Chemical Physics*, **2000**, 112, 220-229	3.9	131
158	Potential energy surfaces for the CN(X 2 ,A 2)Ar system and inelastic scattering within the A state. *Journal of Chemical Physics*, **2000**, 112, 781-791	3.9	47
157	NMR chemical shift calculations within local correlation methods: the GIAO-LMP2 approach. *Physical Chemistry Chemical Physics*, **2000**, 2, 2083-2090	3.6	58
156	Perspective on Theory of self-consistent electron pairs. An iterative method for correlated many-electron wavefunctions **2000**, 322-325		
155	Quartet and sextet states of CS *Journal of Chemical Physics*, **1999**, 110, 11835-11840	3.9	20
154	Integral-direct electron correlation methods. *Molecular Physics*, **1999**, 96, 719-733	1.7	73
153	Impact of local approximations on MP2 vibrational frequencies. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **1999**, 55, 647-658	4.4	71
152	Quantum-mechanical calculation of the thermal rate constant for the H2+Cl->H+HCl reaction. *Chemical Physics Letters*, **1999**, 313, 647-654	2.5	68
151	Local interpolation of ab initio potential energy surfaces for direct dynamics studies of chemical reactions. *Chemical Physics Letters*, **1999**, 302, 208-214	2.5	14

150	The aurophilic attraction as interpreted by local correlation methods. *Journal of Chemical Physics*, **1999**, 110, 7210-7215	3.9	152
149	van der waals interactions in the Cl + HD reaction. *Science*, **1999**, 286, 1713-6	33.3	266
148	Photodissociation dynamics of H2S on new coupled ab initio potential energy surfaces. *Journal of Chemical Physics*, **1999**, 111, 4523-4534	3.9	134
147	Low-order scaling local electron correlation methods. I. Linear scaling local MP2. *Journal of Chemical Physics*, **1999**, 111, 5691-5705	3.9	618
146	Multipole approximation of distant pair energies in local MP2 calculations. *Chemical Physics Letters*, **1998**, 290, 143-149	2.5	167
145	Integral transformation with low-order scaling for large local second-order M□ller-Plesset calculations **1998**, 19, 1241-1254		70
144	Reaction path following by quadratic steepest descent. *Theoretical Chemistry Accounts*, **1998**, 100, 21-30	1.9	43
143	Improved intermolecular water potential from global geometry optimization of small water clusters using local MP2. *Chemical Physics*, **1998**, 239, 561-572	2.3	45
142	Analytical energy gradients for local second-order Mo/ller-Plesset perturbation theory. *Journal of Chemical Physics*, **1998**, 108, 5185-5193	3.9	190
141	Local Treatment of Electron Correlation in Molecular Clusters:´Structures and Stabilities of (H2O)n,n= 2-. *Journal of Physical Chemistry A*, **1998**, 102, 5997-6003	2.8	217
140	Spin-orbit effects in the reaction of F(2P) with H2. *Journal of Chemical Physics*, **1998**, 109, 5710-5713	3.9	116
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