Hans-Joachim Werner

List of Publications by Citations

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	An efficient internally contracted multiconfiguration–reference configuration interaction method. *Journal of Chemical Physics*, **1988**, 89, 5803-5814	3.9	3175
310	A second order multiconfiguration SCF procedure with optimum convergence. *Journal of Chemical Physics*, **1985**, 82, 5053-5063	3.9	2556
309	An efficient method for the evaluation of coupling coefficients in configuration interaction calculations. *Chemical Physics Letters*, **1988**, 145, 514-522	2.5	2327
308	Molpro: a general-purpose quantum chemistry program package. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 242-253	7.9	2254
307	An efficient second-order MC SCF method for long configuration expansions. *Chemical Physics Letters*, **1985**, 115, 259-267	2.5	2210
306	Coupled cluster theory for high spin, open shell reference wave functions. *Journal of Chemical Physics*, **1993**, 99, 5219-5227	3.9	1752
305	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	2.5	1439
304	A simple and efficient CCSD(T)-F12 approximation. *Journal of Chemical Physics*, **2007**, 127, 221106	3.9	1318
303	Simplified CCSD(T)-F12 methods: theory and benchmarks. *Journal of Chemical Physics*, **2009**, 130, 054104	3.9	1272
302	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
301	Spin-orbit matrix elements for internally contracted multireference configuration interaction wavefunctions. *Molecular Physics*, **2000**, 98, 1823-1833	1.7	741
300	Multireference perturbation theory for large restricted and selected active space reference wave functions. *Journal of Chemical Physics*, **2000**, 112, 5546-5557	3.9	690
299	Local treatment of electron correlation in coupled cluster theory. *Journal of Chemical Physics*, **1996**, 104, 6286-6297	3.9	650
298	Low-order scaling local electron correlation methods. I. Linear scaling local MP2. *Journal of Chemical Physics*, **1999**, 111, 5691-5705	3.9	618
297	Combining long-range configuration interaction with short-range density functionals. *Chemical Physics Letters*, **1997**, 275, 151-160	2.5	615
296	Fast linear scaling second-order Møller-Plesset perturbation theory (MP2) using local and density fitting approximations. *Journal of Chemical Physics*, **2003**, 118, 8149-8160	3.9	606
295	PNO-CI and PNO-CEPA studies of electron correlation effects. *Molecular Physics*, **1976**, 31, 855-872	1.7	587

294	Low-order scaling local electron correlation methods. IV. Linear scaling local coupled-cluster (LCCSD). *Journal of Chemical Physics*, **2001**, 114, 661	3.9	521
293	Third-order multireference perturbation theory The CASPT3 method. *Molecular Physics*, **1996**, 89, 645-661	1.7	484
292	General orbital invariant MP2-F12 theory. *Journal of Chemical Physics*, **2007**, 126, 164102	3.9	436
291	Internally contracted multiconfiguration-reference configuration interaction calculations for excited states. *Theoretica Chimica Acta*, **1992**, 84, 95-103		436
290	A quadratically convergent MCSCF method for the simultaneous optimization of several states. *Journal of Chemical Physics*, **1981**, 74, 5794-5801	3.9	399
289	An accurate multireference configuration interaction calculation of the potential energy surface for the F+H2->HF+H reaction. *Journal of Chemical Physics*, **1996**, 104, 6515-6530	3.9	353
288	The self-consistent electron pairs method for multiconfiguration reference state functions. *Journal of Chemical Physics*, **1982**, 76, 3144-3156	3.9	345
287	Finite perturbation calculations for the static dipole polarizabilities of the first-row atoms. *Physical Review A*, **1976**, 13, 13-16	2.6	300
286	A quadratically convergent multiconfiguration□self-consistent field method with simultaneous optimization of orbitals and CI coefficients. *Journal of Chemical Physics*, **1980**, 73, 2342-2356	3.9	298
285	Local perturbative triples correction (T) with linear cost scaling. *Chemical Physics Letters*, **2000**, 318, 370-378	2.8	275
284	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
283	MCSCF study of the avoided curve crossing of the two lowest 1□ states of LiF. *Journal of Chemical Physics*, **1981**, 74, 5802-5807	3.9	272
282	van der waals interactions in the Cl + HD reaction. *Science*, **1999**, 286, 1713-6	33.3	266
281	Magnetic Field Dependence of the Geminate Recombination of Radical Ion Pairs in Polar Solvents. *Zeitschrift Fur Physikalische Chemie*, **1976**, 101, 371-390	3.1	260
280	Fast Hartree□ock theory using local density fitting approximations. *Molecular Physics*, **2004**, 102, 2311-2321	1.7	257
279	Local treatment of electron excitations in the EOM-CCSD method. *Journal of Chemical Physics*, **2003**, 118, 3006-3019	3.9	241
278	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	3.9	239
277	The transition state of the f + h2 reaction. *Science*, **1993**, 262, 1852-5	33.3	234

276	Analytical energy gradients for internally contracted second-order multireference perturbation theory. *Journal of Chemical Physics*, **2003**, 119, 5044-5057	3.9	229
275	First-principles theory for the H + CH4 --> H2 + CH3 reaction. *Science*, **2004**, 306, 2227-9	33.3	227
274	An efficient local coupled cluster method for accurate thermochemistry of large systems. *Journal of Chemical Physics*, **2011**, 135, 144116	3.9	226
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272	High-accuracy computation of reaction barriers in enzymes. *Angewandte Chemie - International Edition*, **2006**, 45, 6856-9	16.4	223
271	Explicitly correlated RMP2 for high-spin open-shell reference states. *Journal of Chemical Physics*, **2008**, 128, 154103	3.9	220
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269	Quantum mechanical angular distributions for the F+H2 reaction. *Journal of Chemical Physics*, **1996**, 104, 6531-6546	3.9	209
268	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
267	Analytical energy gradients for local second-order M ller-Plesset perturbation theory using density fitting approximations. *Journal of Chemical Physics*, **2004**, 121, 737-50	3.9	206
266	The Molpro quantum chemistry package. *Journal of Chemical Physics*, **2020**, 152, 144107	3.9	197
265	Adiabatic and diabatic potential energy surfaces for collisions of CN(X 2, A 2) with He. *Journal of Chemical Physics*, **1988**, 89, 3139-3151	3.9	194
264	Analytical energy gradients for local second-order Mo/llerPlesset perturbation theory. *Journal of Chemical Physics*, **1998**, 108, 5185-5193	3.9	190
263	Explicitly correlated multireference configuration interaction: MRCI-F12. *Journal of Chemical Physics*, **2011**, 134, 034113	3.9	189
262	A new internally contracted multi-reference configuration interaction method. *Journal of Chemical Physics*, **2011**, 135, 054101	3.9	189
261	Low-order scaling local correlation methods II: Splitting the Coulomb operator in linear scaling local second-order M llerPlesset perturbation theory. *Journal of Chemical Physics*, **2000**, 113, 9443-9455	3.9	189
260	Molecular properties from MCSCF-SCEP wave functions. I. Accurate dipole moment functions of OH, OHand OH+. *Journal of Chemical Physics*, **1983**, 79, 905-916	3.9	183
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258	Characterization of the S1/S2 conical intersection in pyrazine using ab initio multiconfiguration self-consistent-field and multireference configuration-interaction methods. *Journal of Chemical Physics*, **1994**, 100, 1400-1413	3.9	176
257	Matrix-Formulated Direct Multiconfiguration Self-Consistent Field and Multiconfiguration Reference Configuration-Interaction Methods. *Advances in Chemical Physics*, **2007**, 1-62		171
256	Explicitly correlated coupled cluster methods with pair-specific geminals. *Molecular Physics*, **2011**, 109, 407-417	1.7	169
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254	A comparison of variational and non-variational internally contracted multiconfiguration-reference configuration interaction calculations. *Theoretica Chimica Acta*, **1991**, 78, 175-187		166
253	Accurate calculation of vibrational frequencies using explicitly correlated coupled-cluster theory. *Journal of Chemical Physics*, **2009**, 130, 054105	3.9	154
252	The aurophilic attraction as interpreted by local correlation methods. *Journal of Chemical Physics*, **1999**, 110, 7210-7215	3.9	152
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250	Third-order multireference perturbation theory The CASPT3 method		149
249	Theory of the magnetic field modulated geminate recombination of radical ion pairs in polar solvents: Application to the pyrene/N,N-dimethylaniline system. *Journal of Chemical Physics*, **1977**, 67, 646-663	3.9	147
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233	Explicitly correlated second-order perturbation theory using density fitting and local approximations. *Journal of Chemical Physics*, **2006**, 124, 054114	3.9	124
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218	Eliminating the domain error in local explicitly correlated second-order Møller-Plesset perturbation theory. *Journal of Chemical Physics*, **2008**, 129, 101103	3.9	102
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214	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
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