Trygve Helgaker

List of Publications by Citations

344 papers	28,100 citations	77 h-index	160 g-index
370 ext. papers	29,765 ext. citations	3.8 avg, IF	6.85 L-index

#	Paper	IF	Citations
344	Basis-set convergence of correlated calculations on water. *Journal of Chemical Physics*, **1997**, 106, 9639-9646	3.9	1932
343	Basis-set convergence in correlated calculations on Ne, N2, and H2O. *Chemical Physics Letters*, **1998**, 286, 243-252	2.5	1786
342	**2000**,		1575
341	Ab Initio Methods for the Calculation of NMR Shielding and Indirect Spinminus signSpin Coupling Constants. *Chemical Reviews*, **1999**, 99, 293-352	68.1	1191
340	Excitation energies in density functional theory: an evaluation and a diagnostic test. *Journal of Chemical Physics*, **2008**, 128, 044118	3.9	1066
339	The Dalton quantum chemistry program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 269-284	7.9	956
338	Basis-set convergence of the energy in molecular HartreeFock calculations. *Chemical Physics Letters*, **1999**, 302, 437-446	2.5	535
337	Excitation energies from the coupled cluster singles and doubles linear response function (CCSDLR). Applications to Be, CH+, CO, and H2O. *Journal of Chemical Physics*, **1990**, 93, 3345-3350	3.9	491
336	Recent advances in wave function-based methods of molecular-property calculations. *Chemical Reviews*, **2012**, 112, 543-631	68.1	453
335	Assessment of a Coulomb-attenuated exchange-correlation energy functional. *Physical Chemistry Chemical Physics*, **2006**, 8, 558-62	3.6	418
334	The CC3 model: An iterative coupled cluster approach including connected triples. *Journal of Chemical Physics*, **1997**, 106, 1808-1818	3.9	362
333	Density-functional theory of linear and nonlinear time-dependent molecular properties. *Journal of Chemical Physics*, **2002**, 117, 9630-9645	3.9	338
332	Basis set convergence of the interaction energy of hydrogen-bonded complexes. *Journal of Chemical Physics*, **1999**, 111, 9157-9167	3.9	333
331	The accurate determination of molecular equilibrium structures. *Journal of Chemical Physics*, **2001**, 114, 6548-6556	3.9	322
330	The prediction of molecular equilibrium structures by the standard electronic wave functions. *Journal of Chemical Physics*, **1997**, 106, 6430-6440	3.9	310
329	Analytical calculation of nuclear magnetic resonance indirect spinSpin coupling constants at the generalized gradient approximation and hybrid levels of density-functional theory. *Journal of Chemical Physics*, **2000**, 113, 9402-9409	3.9	309
328	An electronic Hamiltonian for origin independent calculations of magnetic properties. *Journal of Chemical Physics*, **1991**, 95, 2595-2601	3.9	292

327	Integration of the classical equations of motion on ab initio molecular potential energy surfaces using gradients and Hessians: application to translational energy release upon fragmentation. *Chemical Physics Letters*, **1990**, 173, 145-150	2.5	236
326	The quantum-chemical calculation of NMR indirect spin–spin coupling constants. *Progress in Nuclear Magnetic Resonance Spectroscopy*, **2008**, 53, 249-268	10.4	226
325	Molecular equilibrium structures from experimental rotational constants and calculated vibration–rotation interaction constants. *Journal of Chemical Physics*, **2002**, 116, 6482-6496	3.9	222
324	Coupled cluster energy derivatives. Analytic Hessian for the closed-shell coupled cluster singles and doubles wave function: Theory and applications. *Journal of Chemical Physics*, **1990**, 92, 4924-4940	3.9	214
323	Accuracy of atomization energies and reaction enthalpies in standard and extrapolated electronic wave function/basis set calculations. *Journal of Chemical Physics*, **2000**, 112, 9229-9242	3.9	208
322	Multiconfigurational self-consistent field calculations of nuclear shieldings using London atomic orbitals. *Journal of Chemical Physics*, **1994**, 100, 8178-8185	3.9	208
321	Vibrational Raman optical activity calculations using London atomic orbitals. *Faraday Discussions*, **1994**, 99, 165-180	3.6	206
320	Highly accurate calculations of molecular electronic structure. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1999**, 32, R103-R130	1.3	200
319	A priori calculation of molecular properties to chemical accuracy. *Journal of Physical Organic Chemistry*, **2004**, 17, 913-933	2.1	194
318	A multiconfigurational self-consistent reaction-field method. *Journal of Chemical Physics*, **1988**, 89, 3086-3095	3.9	191
317	Perturbation-dependent atomic orbitals for the calculation of spin-rotation constants and rotational g tensors. *Journal of Chemical Physics*, **1996**, 105, 2804-2812	3.9	182
316	Quantitative quantum chemistry. *Molecular Physics*, **2008**, 106, 2107-2143	1.7	179
315	Optical rotation studied by density-functional and coupled-cluster methods. *Chemical Physics Letters*, **2002**, 352, 533-539	2.5	179
314	Integral-direct coupled cluster calculations of frequency-dependent polarizabilities, transition probabilities and excited-state properties. *Journal of Chemical Physics*, **1998**, 108, 2801-2816	3.9	178
313	Møller–Plesset energy derivatives. *Journal of Chemical Physics*, **1988**, 89, 1560-1570	3.9	176
312	Gauge-origin independent multiconfigurational self-consistent-field theory for vibrational circular dichroism. *Journal of Chemical Physics*, **1993**, 98, 8873-8887	3.9	174
311	Hartree–Fock limit magnetizabilities from London orbitals. *Journal of Chemical Physics*, **1993**, 99, 3847-3859	3.9	174
310	A systematic ab initio study of the water dimer in hierarchies of basis sets and correlation models. *Theoretical Chemistry Accounts*, **1997**, 97, 150-157	1.9	173

309	Large-scale calculations of excitation energies in coupled cluster theory: The singlet excited states of benzene. *Journal of Chemical Physics*, **1996**, 105, 6921-6939	3.9	173
308	Configuration-interaction energy derivatives in a fully variational formulation. *Theoretica Chimica Acta*, **1989**, 75, 111-127		168
307	Basis-set dependence of nuclear spin-spin coupling constants. *Theoretical Chemistry Accounts*, **1998**, 99, 175-182	1.9	165
306	Polarization consistent basis sets. V. The elements Si-Cl. *Journal of Chemical Physics*, **2004**, 121, 3463-70	3.9	164
305	Principles of direct 4-component relativistic SCF: application to caesium auride. *Molecular Physics*, **1997**, 91, 937-950	1.7	152
304	Gauge-Origin Independent Density-Functional Theory Calculations of Vibrational Raman Optical Activity. *Journal of Physical Chemistry A*, **2002**, 106, 7448-7455	2.8	152
303	Analytical Calculation of Geometrical Derivatives in Molecular Electronic Structure Theory. *Advances in Quantum Chemistry*, **1988**, 19, 183-245	1.4	150
302	The integral-direct coupled cluster singles and doubles model. *Journal of Chemical Physics*, **1996**, 104, 4157-4165	3.9	146
301	Vibrational corrections to indirect nuclear spin□spin coupling constants calculated by density-functional theory. *Journal of Chemical Physics*, **2003**, 118, 9572-9581	3.9	144
300	Transition-state optimizations by trust-region image minimization. *Chemical Physics Letters*, **1991**, 182, 503-510	2.5	142
299	Indirect nuclear spin□spin coupling constants from multiconfiguration linear response theory. *Journal of Chemical Physics*, **1992**, 96, 6120-6125	3.9	142
298	Multiconfigurational quadratic response functions for singlet and triplet perturbations: The phosphorescence lifetime of formaldehyde. *Journal of Chemical Physics*, **1992**, 97, 9178-9187	3.9	139
297	The equilibrium structure of ferrocene. *ChemPhysChem*, **2006**, 7, 245-9	3.2	135
296	Four-component relativistic Kohn-Sham theory. *Journal of Computational Chemistry*, **2002**, 23, 814-23	3.5	130
295	Dynamics of the reaction CH2OH+ .fwdarw. CHO+ + H2. Translational energy release from ab initio trajectory calculations. *Journal of the American Chemical Society*, **1992**, 114, 4265-4268	16.4	130
294	Benchmarking two-photon absorption with CC3 quadratic response theory, and comparison with density-functional response theory. *Journal of Chemical Physics*, **2006**, 124, 054322	3.9	125
293	Structural and electronic properties of polyacetylene and polyyne from hybrid and Coulomb-attenuated density functionals. *Journal of Physical Chemistry A*, **2007**, 111, 11930-5	2.8	124
292	Calculations of two-photon absorption cross sections by means of density-functional theory. *Chemical Physics Letters*, **2003**, 374, 446-452	2.5	121

291	Benchmarking density-functional theory calculations of NMR shielding constants and spin-rotation constants using accurate coupled-cluster calculations. *Journal of Chemical Physics*, **2013**, 138, 024111	3.9	119
290	Density functional theory calculation of electronic circular dichroism using London orbitals. *Chemical Physics Letters*, **2004**, 388, 110-119	2.5	119
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286	Coupled-cluster connected quadruples and quintuples corrections to the harmonic vibrational frequencies and equilibrium bond distances of HF, N(2), F(2), and CO. *Journal of Chemical Physics*, **2004**, 121, 5874-84	3.9	110
285	Rovibrational effects, temperature dependence, and isotope effects on the nuclear shielding tensors of water: A new 17O absolute shielding scale. *Journal of Chemical Physics*, **1998**, 109, 8388-8397	3.9	107
284	Molecular Hessians for large-scale MCSCF wave functions. *Journal of Chemical Physics*, **1986**, 84, 6266-6279	3.9	106
283	Basis-set convergence of the molecular electric dipole moment. *Journal of Chemical Physics*, **1999**, 111, 4424-4430	3.9	102
282	Conformational Effects on the Optical Rotation of Alanine and Proline. *Journal of Physical Chemistry A*, **2004**, 108, 4269-4276	2.8	101
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270	Multiple basis sets in calculations of triples corrections in coupled-cluster theory. *Theoretical Chemistry Accounts*, **1997**, 97, 164-176	1.9	79
269	Nonperturbative ab initio calculations in strong magnetic fields using London orbitals. *Journal of Chemical Physics*, **2008**, 129, 154114	3.9	79
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267	Accurate calculation and modeling of the adiabatic connection in density functional theory. *Journal of Chemical Physics*, **2010**, 132, 164115	3.9	77
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204	Current Density Functional Theory Using Meta-Generalized Gradient Exchange-Correlation Functionals. *Journal of Chemical Theory and Computation*, **2015**, 11, 4169-81	6.4	40
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