Trygve Helgaker

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Analytic calculation of the Berry curvature and diagonal Born-Oppenheimer correction for molecular systems in uniform magnetic fields.. *Journal of Chemical Physics*, **2022**, 156, 044121	3.9	6
343	Robust All-Electron Optimization in Orbital-Free Density-Functional Theory Using the Trust-Region Image Method. *Journal of Physical Chemistry A*, **2021**, 125, 459-475	2.8	0
342	Ab Initio molecular dynamics with screened Lorentz forces. II. Efficient propagators and rovibrational spectra in strong magnetic fields. *Journal of Chemical Physics*, **2021**, 155, 024105	3.9	6
341	Ab initio molecular dynamics with screened Lorentz forces. I. Calculation and atomic charge interpretation of Berry curvature. *Journal of Chemical Physics*, **2021**, 155, 024104	3.9	9
340	Lower Semicontinuity of the Universal Functional in Paramagnetic Current-Density Functional Theory. *Journal of Physical Chemistry Letters*, **2021**, 12, 1421-1425	6.4	2
339	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. *Journal of Chemical Physics*, **2020**, 152, 214115	3.9	24
338	Atoms and molecules in soft confinement potentials. *Molecular Physics*, **2020**, 118, e1730989	1.7	8
337	A quantum-mechanical non-Born□Oppenheimer model of a molecule in a strong magnetic field. *Chemical Physics Letters*, **2020**, 761, 138041	2.5	2
336	Bonding in the helium dimer in strong magnetic fields: the role of spin and angular momentum. *Physical Chemistry Chemical Physics*, **2020**, 22, 23502-23521	3.6	9
335	Foreword: Prof. Gauss Festschrift. *Molecular Physics*, **2020**, 118, e1817247	1.7	
334	Analyzing Magnetically Induced Currents in Molecular Systems Using Current-Density-Functional Theory. *Journal of Physical Chemistry A*, **2020**, 124, 1321-1333	2.8	18
333	Challenges for large scale simulation: general discussion. *Faraday Discussions*, **2020**, 224, 309-332	3.6	0
332	New density-functional approximations and beyond: general discussion. *Faraday Discussions*, **2020**, 224, 166-200	3.6	1
331	First-Principles Calculation of H NMR Chemical Shifts of Complex Metal Polyhydrides: The Essential Inclusion of Relativity and Dynamics. *Inorganic Chemistry*, **2020**, 59, 17509-17518	5.1	3
330	Strong correlation in density functional theory: general discussion. *Faraday Discussions*, **2020**, 224, 373-386	3.6	1
329	New approaches to study excited states in density functional theory: general discussion. *Faraday Discussions*, **2020**, 224, 483-508	3.6	2
328	GW quasiparticle energies of atoms in strong magnetic fields. *Journal of Chemical Physics*, **2019**, 150, 214112	3.9	10

327	Kohn-Sham Theory with Paramagnetic Currents: Compatibility and Functional Differentiability. *Journal of Chemical Theory and Computation*, **2019**, 15, 4003-4020	6.4	5
326	Four-component relativistic P NMR calculations for trans-platinum(ii) complexes: importance of the solvent and dynamics in spectral simulations. *Dalton Transactions*, **2019**, 48, 8076-8083	4.3	13
325	KohnSham energy decomposition for molecules in a magnetic field. *Molecular Physics*, **2019**, 117, 97-109	1.7	12
324	Excitation energies from GLevyLevy perturbation theory along the range-separated adiabatic connection. *Molecular Physics*, **2018**, 116, 1443-1451	1.7	4
323	Uniform magnetic fields in density-functional theory. *Journal of Chemical Physics*, **2018**, 148, 024101	3.9	12
322	A computational quantum-mechanical model of a molecular magnetic trap. *Journal of Chemical Physics*, **2018**, 149, 244112	3.9	4
321	Bethe-Salpeter correlation energies of atoms and molecules. *Journal of Chemical Physics*, **2018**, 149, 144106	3.9	16
320	Generalized Kohn-Sham iteration on Banach spaces. *Journal of Chemical Physics*, **2018**, 149, 164103	3.9	5
319	Explicitly-correlated non-born-oppenheimer calculations of the HD molecule in a strong magnetic field. *Chemical Physics Letters*, **2017**, 682, 87-90	2.5	6
318	Connections between variation principles at the interface of wave-function and density-functional theories. *Journal of Chemical Physics*, **2017**, 147, 134107	3.9	3
317	Magnetic-Field Density-Functional Theory (BDFT): Lessons from the Adiabatic Connection. *Journal of Chemical Theory and Computation*, **2017**, 13, 4089-4100	6.4	18
316	A tribute to Jan Erik Almlöf. *Molecular Physics*, **2017**, 115, 2033-2042	1.7	
315	Calculation of NMR Spin-Spin Coupling Constants in Strychnine. *Journal of Organic Chemistry*, **2016**, 81, 11496-11500	4.2	17
314	Alternative Representations of the Correlation Energy in Density-Functional Theory: A Kinetic-Energy Based Adiabatic Connection. *Journal of the Chinese Chemical Society*, **2016**, 63, 121-128	1.5	4
313	Electron localisation function in current-density-functional theory. *Molecular Physics*, **2016**, 114, 1415-1422	1.7	10
312	Nuclei-selected atomic-orbital response-theory formulation for the calculation of NMR shielding tensors using density-fitting. *Journal of Chemical Physics*, **2016**, 145, 234108	3.9	6
311	Comparison of Three Efficient Approximate Exact-Exchange Algorithms: The Chain-of-Spheres Algorithm, Pair-Atomic Resolution-of-the-Identity Method, and Auxiliary Density Matrix Method. *Journal of Chemical Theory and Computation*, **2016**, 12, 3514-22	6.4	21
310	Current Density Functional Theory Using Meta-Generalized Gradient Exchange-Correlation Functionals. *Journal of Chemical Theory and Computation*, **2015**, 11, 4169-81	6.4	40

309	The importance of current contributions to shielding constants in density-functional theory. *Physical Chemistry Chemical Physics*, **2015**, 17, 18834-42	3.6	22
308	Calculating excitation energies by extrapolation along adiabatic connections. *Physical Review A*, **2015**, 91,	2.6	14
307	Molecular properties in the TammDancoff approximation: indirect nuclear spinSpin coupling constants. *Molecular Physics*, **2015**, 113, 1937-1951	1.7	7
306	Fractional Electron Loss in Approximate DFT and Hartree-Fock Theory. *Journal of Chemical Theory and Computation*, **2015**, 11, 5262-8	6.4	33
305	Non-BornDOppenheimer calculations of the HD molecule in a strong magnetic field. *Chemical Physics Letters*, **2015**, 639, 295-299	2.5	9
304	Coupled-cluster theory for atoms and molecules in strong magnetic fields. *Journal of Chemical Physics*, **2015**, 143, 074110	3.9	50
303	Ground-state densities from the Rayleigh-Ritz variation principle and from density-functional theory. *Journal of Chemical Physics*, **2015**, 143, 184106	3.9	7
302	Excited states from range-separated density-functional perturbation theory. *Molecular Physics*, **2015**, 113, 1740-1749	1.7	11
301	Geometry of the magic number H(+)(H2O)21 water cluster by proxy. *Physical Chemistry Chemical Physics*, **2015**, 17, 5466-73	3.6	7
300	Use of density functional theory orbitals in the GVVPT2 variant of second-order multistate multireference perturbation theory. *Journal of Physical Chemistry A*, **2015**, 119, 1548-53	2.8	9
299	Excitation energies from ensemble DFT **2015**,		2
298	The Dalton quantum chemistry program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 269-284	7.9	956
297	Excitation energies along a range-separated adiabatic connection. *Journal of Chemical Physics*, **2014** , 141, 044123	3.9	17
296	Charge-constrained auxiliary-density-matrix methods for the Hartree-Fock exchange contribution. *Journal of Chemical Physics*, **2014**, 141, 094104	3.9	15
295	Analytic cubic and quartic force fields using density-functional theory. *Journal of Chemical Physics*, **2014**, 140, 034103	3.9	34
294	Mechanochemistry: the effect of dynamics. *Journal of Physical Chemistry A*, **2014**, 118, 7683-94	2.8	19
293	Differentiable but exact formulation of density-functional theory. *Journal of Chemical Physics*, **2014** , 140, 18A518	3.9	31
292	Multiconfigurational Self-Consistent Field Theory **2014**, 598-647		2

291	Short-Range Interactions and Orbital Expansions **2014**, 256-286		2
290	Gaussian Basis Sets **2014**, 287-335		1
289	Coupled-Cluster Theory **2014**, 648-723		5
288	Molecular Integral Evaluation **2014**, 336-432		4
287	Calibration of the Electronic-Structure Models **2014**, 817-883		7
286	Non-perturbative calculation of molecular magnetic properties within current-density functional theory. *Journal of Chemical Physics*, **2014**, 140, 034101	3.9	43
285	Fermion N-representability for prescribed density and paramagnetic current density. *Physical Review A*, **2014**, 89,	2.6	11
284	A theoretical study on the hydrogen transport mechanism in SrTiO3 perovskite. II. Scandium doping at titanium site. *International Journal of Quantum Chemistry*, **2013**, 113, 599-604	2.1	3
283	Communication: Analytic gradients in the random-phase approximation. *Journal of Chemical Physics* , **2013**, 139, 081101	3.9	34
282	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
281	Attractive electron-electron interactions within robust local fitting approximations. *Journal of Computational Chemistry*, **2013**, 34, 1486-96	3.5	52
280	Internal-to-Cartesian back transformation of molecular geometry steps using high-order geometric derivatives. *Journal of Computational Chemistry*, **2013**, 34, 1842-9	3.5	4
279	The accuracy of the Gaussian-and-finite-element-Coulomb (GFC) method for the calculation of Coulomb integrals. *Journal of Chemical Physics*, **2013**, 139, 054114	3.9	2
278	33S hyperfine interactions in H2S and SO2 and revision of the sulfur nuclear magnetic shielding scale. *Journal of Chemical Physics*, **2013**, 139, 244308	3.9	21
277	Insights into the dynamics of evaporation and proton migration in protonated water clusters from large-scale Born-Oppenheimer direct dynamics. *Journal of Computational Chemistry*, **2013**, 34, 533-44	3.5	7
276	Alternative separation of exchange and correlation energies in multi-configuration range-separated density-functional theory. *Journal of Chemical Physics*, **2013**, 139, 134113	3.9	30
275	A Theoretical Study on Proton Conduction Mechanism in BaZrO3 Perovskite. *Progress in Theoretical Chemistry and Physics*, **2013**, 233-248	0.6	6
274	The NMR indirect nuclear spin–spin coupling constant of the HD molecule. *Molecular Physics*, **2012**, 110, 2611-2617	1.7	12

273	Analytical GIAO and hybrid-basis integral derivatives: application to geometry optimization of molecules in strong magnetic fields. *Physical Chemistry Chemical Physics*, **2012**, 14, 9492-9	3.6	31
272	A paramagnetic bonding mechanism for diatomics in strong magnetic fields. *Science*, **2012**, 337, 327-31	33.3	94
271	A theoretical study on hydrogen transport mechanism in SrTio3 perovskite. *International Journal of Quantum Chemistry*, **2012**, 112, 201-207	2.1	5
270	Multi-electron integrals. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 290-303	7.9	44
269	Recent advances in wave function-based methods of molecular-property calculations. *Chemical Reviews*, **2012**, 112, 543-631	68.1	453
268	Calculation of the two-electron Darwin term using explicitly correlated wave functions. *Chemical Physics*, **2012**, 401, 146-151	2.3	2
267	Choice of basic variables in current-density-functional theory. *Physical Review A*, **2012**, 86,	2.6	34
266	Influence of external force on properties and reactivity of disulfide bonds. *Journal of Physical Chemistry A*, **2011**, 115, 2308-15	2.8	43
265	Dispersion interactions in density-functional theory: an adiabatic-connection analysis. *Journal of Chemical Physics*, **2011**, 135, 194109	3.9	18
264	The ab initio calculation of molecular electric, magnetic and geometric properties. *Physical Chemistry Chemical Physics*, **2011**, 13, 2627-51	3.6	55
263	Relativistic four-component calculations of Buckingham birefringence using London atomic orbitals. *Theoretical Chemistry Accounts*, **2011**, 129, 685-699	1.9	4
262	Spin flipping in ring-coupled-cluster-doubles theory. *Chemical Physics Letters*, **2011**, 510, 147-153	2.5	41
261	Range-dependent adiabatic connections. *Journal of Chemical Physics*, **2010**, 133, 164112	3.9	29
260	An efficient density-functional-theory force evaluation for large molecular systems. *Journal of Chemical Physics*, **2010**, 133, 044102	3.9	19
259	Accurate calculation and modeling of the adiabatic connection in density functional theory. *Journal of Chemical Physics*, **2010**, 132, 164115	3.9	77
258	Spin–spin coupling constants and triplet instabilities in Kohn–Sham theory. *Molecular Physics*, **2010**, 108, 2579-2590	1.7	40
257	Benchmarking density-functional-theory calculations of rotational g tensors and magnetizabilities using accurate coupled-cluster calculations. *Journal of Chemical Physics*, **2009**, 131, 144104	3.9	47
256	Implementation of the incremental scheme for one-electron first-order properties in coupled-cluster theory. *Journal of Chemical Physics*, **2009**, 131, 154102	3.9	34

255	The geminal basis in explicitly correlated wave functions. *Chemical Physics*, **2009**, 356, 25-30	2.3	24
254	Robust and Reliable Multilevel Minimization of the Kohn-Sham Energy. *Journal of Chemical Theory and Computation*, **2009**, 5, 1027-32	6.4	12
253	The calculation of adiabatic-connection curves from full configuration-interaction densities: two-electron systems. *Journal of Chemical Physics*, **2009**, 130, 104111	3.9	59
252	Assessment of theoretical methods for the determination of the mechanochemical strength of covalent bonds. *Molecular Physics*, **2009**, 107, 2537-2546	1.7	41
251	Non-perturbative magnetic phenomena in closed-shell paramagnetic molecules. *Physical Chemistry Chemical Physics*, **2009**, 11, 5489-98	3.6	53
250	A stepwise atomic, valence-molecular, and full-molecular optimisation of the Hartree-Fock/Kohn-Sham energy. *Physical Chemistry Chemical Physics*, **2009**, 11, 5805-13	3.6	13
249	Hartree-Fock and Kohn-Sham time-dependent response theory in a second-quantization atomic-orbital formalism suitable for linear scaling. *Journal of Chemical Physics*, **2008**, 129, 054106	3.9	41
248	Maps of current density using density-functional methods. *Journal of Chemical Physics*, **2008**, 129, 074101	3.9	45
247	Quantitative quantum chemistry. *Molecular Physics*, **2008**, 106, 2107-2143	1.7	179
246	Variational and robust density fitting of four-center two-electron integrals in local metrics. *Journal of Chemical Physics*, **2008**, 129, 104101	3.9	71
245	A ground-state-directed optimization scheme for the Kohn-Sham energy. *Physical Chemistry Chemical Physics*, **2008**, 10, 5344-8	3.6	14
244	Second-order Møller-Plesset calculations on the water molecule using Gaussian-type orbital and Gaussian-type geminal theory. *Physical Chemistry Chemical Physics*, **2008**, 10, 3377-82	3.6	10
243	Nonperturbative ab initio calculations in strong magnetic fields using London orbitals. *Journal of Chemical Physics*, **2008**, 129, 154114	3.9	79
242	Efficient elimination of response parameters in molecular property calculations for variational and nonvariational energies. *Journal of Chemical Physics*, **2008**, 129, 214103	3.9	33
241	Density-functional calculations of the nuclear magnetic shielding and indirect nuclear spin–spin coupling constants of three isomers of C20. *Molecular Physics*, **2008**, 106, 2357-2365	1.7	2
240	The augmented Roothaan-Hall method for optimizing Hartree-Fock and Kohn-Sham density matrices. *Journal of Chemical Physics*, **2008**, 129, 124106	3.9	37
239	The quantum-chemical calculation of NMR indirect spin–spin coupling constants. *Progress in Nuclear Magnetic Resonance Spectroscopy*, **2008**, 53, 249-268	10.4	226
238	Static and frequency-dependent dipole-dipole polarizabilities of all closed-shell atoms up to radium: a four-component relativistic DFT study. *ChemPhysChem*, **2008**, 9, 445-53	3.2	26

237	Excitation energies in density functional theory: an evaluation and a diagnostic test. *Journal of Chemical Physics*, **2008**, 128, 044118	3.9	1066
236	Accurate quantum-chemical calculations using Gaussian-type geminal and Gaussian-type orbital basis sets: applications to atoms and diatomics. *Physical Chemistry Chemical Physics*, **2007**, 9, 3112-26	3.6	39
235	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
234	Electron correlation: the many-body problem at the heart of chemistry. *Journal of Computational Chemistry*, **2007**, 28, 1307-20	3.5	69
233	Electronic circular dichroism of disulphide bridge: ab initio quantum-chemical calculations. *Journal of Chemical Physics*, **2007**, 127, 085102	3.9	17
232	Linear-scaling implementation of molecular electronic self-consistent field theory. *Journal of Chemical Physics*, **2007**, 126, 114110	3.9	71
231	Linear-scaling implementation of molecular response theory in self-consistent field electronic-structure theory. *Journal of Chemical Physics*, **2007**, 126, 154108	3.9	83
230	A unified scheme for the calculation of differentiated and undifferentiated molecular integrals over solid-harmonic Gaussians. *Physical Chemistry Chemical Physics*, **2007**, 9, 4771-9	3.6	31
229	Density-Functional and Coupled-Cluster Singles-and-Doubles Calculations of the Nuclear Shielding and Indirect Nuclear Spin-Spin Coupling Constants of o-Benzyne. *Journal of Chemical Theory and Computation*, **2007**, 3, 86-94	6.4	40
228	Linear-scaling symmetric square-root decomposition of the overlap matrix. *Journal of Chemical Physics*, **2007**, 126, 124104	3.9	36
227	The equilibrium structure of ferrocene. *ChemPhysChem*, **2006**, 7, 245-9	3.2	135
226	A second-quantization framework for the unified treatment of relativistic and nonrelativistic molecular perturbations by response theory. *Journal of Chemical Physics*, **2006**, 125, 24102	3.9	3
225	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
224	The magnetizability, rotational g tensor and quadrupole moment of the boron trihalides. *Molecular Physics*, **2006**, 104, 847-856	1.7	4
223	Assessment of a Coulomb-attenuated exchange-correlation energy functional. *Physical Chemistry Chemical Physics*, **2006**, 8, 558-62	3.6	418
222	Rotational g Tensors Calculated Using Hybrid Exchange-Correlation Functionals with the Optimized Effective Potential Approach. *Journal of Chemical Theory and Computation*, **2006**, 2, 827-34	6.4	14
221	Density-functional-theory study of the electric-field-induced second harmonic generation (EFISHG) of push–pull phenylpolyenes in solution. *Chemical Physics Letters*, **2006**, 425, 267-272	2.5	96
220	Choice of exchange-correlation functional for computing NMR indirect spin–spin coupling constants. *Chemical Physics Letters*, **2006**, 425, 163-166	2.5	53

219	Towards black-box linear scaling optimization in Hartree-Fock and Kohn-Sham theories **2006**, 177-189		
218	Calculations of two-photon charge-transfer excitations using Coulomb-attenuated density-functional theory. *Journal of Chemical Physics*, **2005**, 123, 184108	3.9	97
217	A comparison of density-functional-theory and coupled-cluster frequency-dependent polarizabilities and hyperpolarizabilities. *Molecular Physics*, **2005**, 103, 439-450	1.7	69
216	Theoretical studies of nuclear magnetic resonance parameters for the proton-exchange pathways in porphyrin and porphycene. *Journal of Physical Chemistry A*, **2005**, 109, 4162-71	2.8	22
215	The Rotational g Tensor as a Benchmark for Density-Functional Theory Calculations of Molecular Magnetic Properties. *Journal of Chemical Theory and Computation*, **2005**, 1, 877-88	6.4	23
214	Atmospheric chemistry of CHF2CHO: study of the IR and UV-vis absorption cross sections, photolysis, and OH-, Cl-, and NO3-initiated oxidation. *Journal of Physical Chemistry A*, **2005**, 109, 3652-62	2.8	7
213	Quadratic response functions in a second-order polarization propagator framework. *Journal of Physical Chemistry A*, **2005**, 109, 11618-28	2.8	26
212	The Rotational g Tensor as a Benchmark for Ab Initio Molecular Property Calculations. *Advances in Quantum Chemistry*, **2005**, 77-90	1.4	4
211	Linear response at the 4-component relativistic density-functional level: application to the frequency-dependent dipole polarizability of Hg, AuH and PtH2. *Chemical Physics*, **2005**, 311, 187-201	2.3	66
210	The accuracy of ab initio molecular geometries for systems containing second-row atoms. *Journal of Chemical Physics*, **2005**, 123, 184107	3.9	113
209	A computational study of some electric and magnetic properties of gaseous BF3 and BCl3. *Journal of Chemical Physics*, **2005**, 123, 114307	3.9	8
208	The trust-region self-consistent field method in Kohn-Sham density-functional theory. *Journal of Chemical Physics*, **2005**, 123, 074103	3.9	28
207	Density-functional theory study of electric and magnetic properties of hexafluorobenzene in the vapor phase. *Journal of Chemical Physics*, **2005**, 122, 234314	3.9	25
206	First-order relativistic corrections to response properties: the hyperpolarizability of the Ne atom. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2004**, 37, 3753-3763	1.3	21
205	A closed-shell coupled-cluster treatment of the Breit-Pauli first-order relativistic energy correction. *Journal of Chemical Physics*, **2004**, 121, 6591-8	3.9	24
204	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
203	Calculation of electric dipole hypershieldings at the nuclei in the Hellmann-Feynman approximation. *Journal of Chemical Physics*, **2004**, 120, 3142-51	3.9	11
202	Polarization consistent basis sets. V. The elements Si-Cl. *Journal of Chemical Physics*, **2004**, 121, 3463-70	3.9	164

201	The expansion of hydrogen states in Gaussian orbitals. *Theoretical Chemistry Accounts*, **2004**, 112, 124	1.9	4
200	A priori calculation of molecular properties to chemical accuracy. *Journal of Physical Organic Chemistry*, **2004**, 17, 913-933	2.1	194
199	The performance of hybrid density functional theory for the calculation of indirect nuclear spin-spin coupling constants in substituted hydrocarbons. *Magnetic Resonance in Chemistry*, **2004**, 42 Spec no, S117-27	2.1	65
198	The calculation of indirect nuclear spin-spin coupling constants in large molecules. *Chemistry - A European Journal*, **2004**, 10, 4627-39	4.8	35
197	The NMR indirect nuclear spin–spin coupling constants for some small rigid hydrocarbons: molecular equilibrium values and vibrational corrections. *Chemical Physics*, **2004**, 296, 53-62	2.3	55
196	Density functional theory calculation of electronic circular dichroism using London orbitals. *Chemical Physics Letters*, **2004**, 388, 110-119	2.5	119
195	GIAO shielding constants and indirect spin–spin coupling constants: performance of density functional methods. *Chemical Physics Letters*, **2004**, 391, 374-379	2.5	78
194	The trust-region self-consistent field method: towards a black-box optimization in Hartree-Fock and Kohn-Sham theories. *Journal of Chemical Physics*, **2004**, 121, 16-27	3.9	59
193	Conformational Effects on the Optical Rotation of Alanine and Proline. *Journal of Physical Chemistry A*, **2004**, 108, 4269-4276	2.8	101
192	Density-functional theory calculations of optical rotatory dispersion in the nonresonant and resonant frequency regions. *Journal of Chemical Physics*, **2004**, 120, 5027-35	3.9	72
191	Potential Energy and Spin–Spin Coupling Constants Surface of Glycolaldehyde. *Journal of Physical Chemistry A*, **2004**, 108, 2758-2769	2.8	18
190	A comparison of polarization and bond functions for density functional calculations. *Molecular Physics*, **2004**, 102, 2559-2562	1.7	3
189	Spin–Spin Coupling Constants with HF and DFT Methods **2004**, 101-121		22
188	Linear-scaling formation of Kohn-Sham Hamiltonian: application to the calculation of excitation energies and polarizabilities of large molecular systems. *Journal of Chemical Physics*, **2004**, 121, 2915-31	3.9	49
187	Density-functional generalized-gradient and hybrid calculations of electromagnetic properties using Slater basis sets. *Journal of Chemical Physics*, **2004**, 120, 7252-61	3.9	25
186	Models of fragmentations induced by electron attachment to protonated peptides. *European Journal of Mass Spectrometry*, **2004**, 10, 625-38	1.1	56
185	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
184	Coupled-cluster connected-quadruples corrections to atomization energies. *Chemical Physics Letters*, **2003**, 371, 62-67	2.5	65

183	Sternheimer shieldings and EFG polarizabilities: a density-functional theory study. *Chemical Physics Letters*, **2003**, 372, 377-385	2.5	4
182	Calculations of hydrogen-bond-transmitted indirect nuclear spin□spin couplings: a comparison of density-functional and ab initio methods. *Chemical Physics Letters*, **2003**, 372, 476-484	2.5	27
181	Calculations of two-photon absorption cross sections by means of density-functional theory. *Chemical Physics Letters*, **2003**, 374, 446-452	2.5	121
180	Characterization of dihydrogen-bonded D□H?H□A complexes on the basis of infrared and magnetic resonance spectroscopic parameters. *Journal of Chemical Physics*, **2003**, 119, 5094-5104	3.9	62
179	The Spin□Spin Coupling Constants in Ethane, Methanol and Methylamine: A Comparison of DFT, MCSCF and CCSD Results. *International Journal of Molecular Sciences*, **2003**, 4, 143-157	6.3	37
178	Density-functional theory calculation of the nuclear magnetic resonance indirect nuclear spin□spin coupling constants in C60. *Molecular Physics*, **2003**, 101, 1997-2002	1.7	15
177	Density functional theory of nonlinear triplet response properties with applications to phosphorescence. *Journal of Chemical Physics*, **2003**, 119, 11024-11034	3.9	76
176	Accuracy of spectroscopic constants of diatomic molecules from ab initio calculations. *Journal of Chemical Physics*, **2003**, 118, 2539	3.9	69
175	A Lagrangian, integral-density direct formulation and implementation of the analytic CCSD and CCSD(T) gradients. *Journal of Chemical Physics*, **2003**, 118, 2985-2998	3.9	54
174	Automated calculation of fundamental frequencies: Application to AlH3 using the coupled-cluster singles-and-doubles with perturbative triples method. *Journal of Chemical Physics*, **2003**, 119, 1951-1960	3.9	71
173	Four-component relativistic Kohn-Sham theory. *Journal of Computational Chemistry*, **2002**, 23, 814-23	3.5	130
172	Software news and updates. Basis-set completeness profiles in two dimensions. *Journal of Computational Chemistry*, **2002**, 23, 420-5	3.5	9
171	Second-order M□ller□Plesset perturbation theory with terms linear in the interelectronic coordinates and exact evaluation of three-electron integrals. *Theoretical Chemistry Accounts*, **2002**, 107, 173-179	1.9	40
170	Computation of two-electron Gaussian integrals for wave functions including the correlation factor r12exp(□122). *Computer Physics Communications*, **2002**, 149, 1-10	4.2	37
169	Optical rotation studied by density-functional and coupled-cluster methods. *Chemical Physics Letters*, **2002**, 352, 533-539	2.5	179
168	Parity-violating interaction in H2O2 calculated from density-functional theory. *Chemical Physics Letters*, **2002**, 354, 274-282	2.5	39
167	Vibronic transitions from coupled-cluster response theory: Theory and application to HSiF and H[sub 2]O. *Journal of Chemical Physics*, **2002**, 116, 8334	3.9	8
166	Molecular equilibrium structures from experimental rotational constants and calculated vibration□otation interaction constants. *Journal of Chemical Physics*, **2002**, 116, 6482-6496	3.9	222

165	Gauge-Origin Independent Density-Functional Theory Calculations of Vibrational Raman Optical Activity. *Journal of Physical Chemistry A*, **2002**, 106, 7448-7455	2.8	152
164	The efficient optimization of molecular geometries using redundant internal coordinates. *Journal of Chemical Physics*, **2002**, 117, 9160-9174	3.9	88
163	Spin–spin coupling tensors by density-functional linear response theory. *Journal of Chemical Physics* , **2002**, 117, 5998-6009	3.9	66
162	Density-functional theory of linear and nonlinear time-dependent molecular properties. *Journal of Chemical Physics*, **2002**, 117, 9630-9645	3.9	338
161	Efficient evaluation of one-center three-electron Gaussian integrals. *Theoretical Chemistry Accounts* , **2001**, 106, 280-286	1.9	18
160	Chemical accuracy from Coulomb hole–extrapolated molecular quantum-mechanical calculations. *Journal of Molecular Structure*, **2001**, 567-568, 375-384	3.4	37
159	Geometrical derivatives and magnetic properties in atomic-orbital density-based Hartree–Fock theory. *Journal of Chemical Physics*, **2001**, 115, 10344	3.9	32
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