Trygve Helgaker

List of Publications by Year
in descending order

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349 papers	31,566 citations	6254 80 h-index	5679 162 g-index
371 all docs	371 docs citations	371 times ranked	12106 citing authors

#	Article	IF	Citations
1	Basis-set convergence of correlated calculations on water. Journal of Chemical Physics, 1997, 106, 9639-9646.	3.0	2,197
2	Basis-set convergence in correlated calculations on Ne, N2, and H2O. Chemical Physics Letters, 1998, 286, 243-252.	2.6	1,989
3	Ab Initio Methods for the Calculation of NMR Shielding and Indirect Spinâ^'Spin Coupling Constants. Chemical Reviews, 1999, 99, 293-352.	47.7	1,318
4	Excitation energies in density functional theory: An evaluation and a diagnostic test. Journal of Chemical Physics, 2008, 128, 044118.	3.0	1,190
5	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	14.6	1,166
6	Basis-set convergence of the energy in molecular Hartreeâ€“Fock calculations. Chemical Physics Letters, 1999, 302, 437-446.	2.6	604
7	Recent Advances in Wave Function-Based Methods of Molecular-Property Calculations. Chemical Reviews, 2012, 112, 543-631.	47.7	549
8	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.	3.0	529
9	Assessment of a Coulomb-attenuated exchangeâ€“correlation energy functional. Physical Chemistry Chemical Physics, 2006, 8, 558-562.	2.8	437
10	The CC3 model: An iterative coupled cluster approach including connected triples. Journal of Chemical Physics, 1997, 106, 1808-1818.	3.0	412
11	Basis set convergence of the interaction energy of hydrogen-bonded complexes. Journal of Chemical Physics, 1999, 111, 9157-9167.	3.0	363
12	Density-functional theory of linear and nonlinear time-dependent molecular properties. Journal of Chemical Physics, 2002, 117, 9630-9645.	3.0	359
13	The accurate determination of molecular equilibrium structures. Journal of Chemical Physics, 2001, 114, 6548-6556.	3.0	353
14	Analytical calculation of nuclear magnetic resonance indirect spinâ€“spin coupling constants at the generalized gradient approximation and hybrid levels of density-functional theory. Journal of Chemical Physics, 2000, 113, 9402-9409.	3.0	345
15	The prediction of molecular equilibrium structures by the standard electronic wave functions. Journal of Chemical Physics, 1997, 106, 6430-6440.	3.0	333
16	An electronic Hamiltonian for origin independent calculations of magnetic properties. Journal of Chemical Physics, 1991, 95, 2595-2601.	3.0	320
17	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.	2.6	254
18	The quantum-chemical calculation of NMR indirect spinâ€“spin coupling constants. Progress in Nuclear Magnetic Resonance Spectroscopy, 2008, 53, 249-268.	7.5	252

#	Article	IF	Citations
19	Molecular equilibrium structures from experimental rotational constants and calculated vibrationâ€“rotation interaction constants. Journal of Chemical Physics, 2002, 116, 6482-6496.	3.0	245
20	Multiconfigurational selfâ€consistent field calculations of nuclear shieldings using London atomic orbitals. Journal of Chemical Physics, 1994, 100, 8178-8185.	3.0	229
21	Vibrational Raman optical activity calculations using London atomic orbitals. Faraday Discussions, 1994, 99, 165-180.	3.2	225
22	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.	3.0	224
23	Coupled cluster energy derivatives. Analytic Hessian for the closedâ€shell coupled cluster singles and doubles wave function: Theory and applications. Journal of Chemical Physics, 1990, 92, 4924-4940.	3.0	222
24	Quantitative quantum chemistry. Molecular Physics, 2008, 106, 2107-2143.	1.7	215
25	Highly accurate calculations of molecular electronic structure. Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, R103-R130.	1.5	214
26	A priori calculation of molecular properties to chemical accuracy. Journal of Physical Organic Chemistry, 2004, 17, 913-933.	1.9	204
27	Hartreeâ€“Fock limit magnetizabilities from London orbitals. Journal of Chemical Physics, 1993, 99, 3847-3859.	3.0	202
28	Perturbationâ€dependent atomic orbitals for the calculation of spinâ€rotation constants and rotational g tensors. Journal of Chemical Physics, 1996, 105, 2804-2812.	3.0	201
29	A multiconfigurational selfâ€consistent reactionâ€field method. Journal of Chemical Physics, 1988, 89, 3086-3095.	3.0	198
30	Optical rotation studied by density-functional and coupled-cluster methods. Chemical Physics Letters, 2002, 352, 533-539.	2.6	192
31	Integral-direct coupled cluster calculations of frequency-dependent polarizabilities, transition probabilities and excited-state properties. Journal of Chemical Physics, 1998, 108, 2801-2816.	3.0	191
32	Mo/llerâ€“Plesset energy derivatives. Journal of Chemical Physics, 1988, 89, 1560-1570.	3.0	190
33	Configuration-interaction energy derivatives in a fully variational formulation. Theoretica Chimica Acta, 1989, 75, 111-127.	0.8	186
34	Gaugeâ€origin independent multiconfigurational selfâ€consistentâ€field theory for vibrational circular dichroism. Journal of Chemical Physics, 1993, 98, 8873-8887.	3.0	186
35	A systematic ab initio study of the water dimer in hierarchies of basis sets and correlation models. Theoretical Chemistry Accounts, 1997, 97, 150-157.	1.4	184
36	Largeâ€scale calculations of excitation energies in coupled cluster theory: The singlet excited states of benzene. Journal of Chemical Physics, 1996, 105, 6921-6939.	3.0	182

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37	Polarization consistent basis sets. V. The elements Siâ€“Cl. Journal of Chemical Physics, 2004, 121, 3463-3470.	3.0	181
38	Basis-set dependence of nuclear spin-spin coupling constants. Theoretical Chemistry Accounts, 1998, 99, 175-182.	1.4	175
39	Principles of direct 4-component relativistic SCF: application to caesium auride. Molecular Physics, 1997, 91, 937-950.	1.7	169
40	Analytical Calculation of Geometrical Derivatives in Molecular Electronic Structure Theory. Advances in Quantum Chemistry, 1988, 19, 183-245.	0.8	167
41	Gauge-Origin Independent Density-Functional Theory Calculations of Vibrational Raman Optical Activity. Journal of Physical Chemistry A, 2002, 106, 7448-7455.	2.5	162
42	Transition-state optimizations by trust-region image minimization. Chemical Physics Letters, 1991, 182, 503-510.	2.6	156
43	Vibrational corrections to indirect nuclear spinâ€“spin coupling constants calculated by density-functional theory. Journal of Chemical Physics, 2003, 118, 9572-9581.	3.0	156
44	The integralâ€direct coupled cluster singles and doubles model. Journal of Chemical Physics, 1996, 104, 4157-4165.	3.0	154
45	Benchmarking density-functional theory calculations of NMR shielding constants and spinâ€“rotation constants using accurate coupled-cluster calculations. Journal of Chemical Physics, 2013, 138, 024111.	3.0	153
46	The Equilibrium Structure of Ferrocene. ChemPhysChem, 2006, 7, 245-249.	2.1	149
47	Multiconfigurational quadratic response functions for singlet and triplet perturbations: The phosphorescence lifetime of formaldehyde. Journal of Chemical Physics, 1992, 97, 9178-9187.	3.0	148
48	Indirect nuclear spinâ€“spin coupling constants from multiconfiguration linear response theory. Journal of Chemical Physics, 1992, 96, 6120-6125.	3.0	147
49	Four-component relativistic Kohn-Sham theory. Journal of Computational Chemistry, 2002, 23, 814-823.	3.3	147
50	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.	13.7	141
51	Structural and Electronic Properties of Polyacetylene and Polyyne from Hybrid and Coulomb-Attenuated Density Functionals. Journal of Physical Chemistry A, 2007, 111, 11930-11935.	2.5	139
52	Benchmarking two-photon absorption with CC3 quadratic response theory, and comparison with density-functional response theory. Journal of Chemical Physics, 2006, 124, 054322.	3.0	137
53	Calculations of two-photon absorption cross sections by means of density-functional theory. Chemical Physics Letters, 2003, 374, 446-452.	2.6	136
54	A direct atomic orbital driven implementation of the coupled cluster singles and doubles (CCSD) model. Chemical Physics Letters, 1994, 228, 233-238.	2.6	126

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55	Coupled-cluster connected quadruples and quintuples corrections to the harmonic vibrational frequencies and equilibrium bond distances of HF, N2, F2, and CO. Journal of Chemical Physics, 2004, 121, 5874-5884.	3.0	125
56	The accuracy ofab initiomolecular geometries for systems containing second-row atoms. Journal of Chemical Physics, 2005, 123, 184107.	3.0	125
57	Density functional theory calculation of electronic circular dichroism using London orbitals. Chemical Physics Letters, 2004, 388, 110-119.	2.6	123
58	A Paramagnetic Bonding Mechanism for Diatomics in Strong Magnetic Fields. Science, 2012, 337, 327-331.	12.6	123
59	First-order one-electron properties in the integral-direct coupled cluster singles and doubles model. Journal of Chemical Physics, 1997, 107, 849-866.	3.0	122
60	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.	3.0	115
61	Basis-set convergence of the molecular electric dipole moment. Journal of Chemical Physics, 1999, 111, 4424-4430.	3.0	114
62	Calculations of two-photon charge-transfer excitations using Coulomb-attenuated density-functional theory. Journal of Chemical Physics, 2005, 123, 184108.	3.0	112
63	Molecular Hessians for largeâ€scale MCSCF wave functions. Journal of Chemical Physics, 1986, 84, 6266-6279.	3.0	109
64	The efficient optimization of molecular geometries using redundant internal coordinates. Journal of Chemical Physics, 2002, 117, 9160-9174.	3.0	109
65	Nuclear shielding constants by density functional theory with gauge including atomic orbitals. Journal of Chemical Physics, 2000, 113, 2983-2989.	3.0	104
66	Conformational Effects on the Optical Rotation of Alanine and Proline. Journal of Physical Chemistry A, 2004, 108, 4269-4276.	2.5	103
67	Density-functional-theory study of the electric-field-induced second harmonic generation (EFISHG) of pushâ€“pull phenylpolyenes in solution. Chemical Physics Letters, 2006, 425, 267-272.	2.6	99
68	Nonperturbative ab initio calculations in strong magnetic fields using London orbitals. Journal of Chemical Physics, 2008, 129, 154114.	3.0	99
69	The molecular structure of ferrocene. Journal of Chemical Physics, 1996, 104, 9528-9530.	3.0	98
70	Direct atomic orbital based selfâ€consistentâ€field calculations of nonlinear molecular properties. Application to the frequency dependent hyperpolarizability of paraâ€nitroaniline. Journal of Chemical Physics, 1993, 98, 6417-6423.	3.0	94
71	A numerically stable procedure for calculating Mï¿½ller-Plesset energy derivatives, derived using the theory of Lagrangians. Theoretica Chimica Acta, 1989, 76, 227-245.	0.8	92
72	Spinâ€“orbit coupling constants in a multiconfiguration linear response approach. Journal of Chemical Physics, 1992, 96, 2118-2126.	3.0	90

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73	Electric field dependence of magnetic properties: Multiconfigurational selfâ€consistent field calculations of hypermagnetizabilities and nuclear shielding polarizabilities of N2, C2H2, HCN, and H2O. Journal of Chemical Physics, 1995, 102, 8953-8966.	3.0	89
74	GIAO shielding constants and indirect spinâ€“spin coupling constants: performance of density functional methods. Chemical Physics Letters, 2004, 391, 374-379.	2.6	87
75	Linear-scaling implementation of molecular response theory in self-consistent field electronic-structure theory. Journal of Chemical Physics, 2007, 126, 154108.	3.0	87
76	Accurate calculation and modeling of the adiabatic connection in density functional theory. Journal of Chemical Physics, 2010, 132, 164115.	3.0	86
77	Ab initio. Theoretica Chimica Acta, 1995, 90, 441.	0.8	86
78	A second-quantization approach to the analytical evaluation of response properties for perturbation-dependent basis sets. International Journal of Quantum Chemistry, 1984, 26, 275-291.	2.0	82
79	Multiple basis sets in calculations of triples corrections in coupled-cluster theory. Theoretical Chemistry Accounts, 1997, 97, 164-176.	1.4	82
80	Electron correlation: The many-body problem at the heart of chemistry. Journal of Computational Chemistry, 2007, 28, 1307-1320.	3.3	82
81	Density-functional theory calculations of optical rotatory dispersion in the nonresonant and resonant frequency regions. Journal of Chemical Physics, 2004, 120, 5027-5035.	3.0	81
82	Divergence in MÃ¸llerâ€“Plesset theory: A simple explanation based on a two-state model. Journal of Chemical Physics, 2000, 112, 9736-9748.	3.0	79
83	Density functional theory of nonlinear triplet response properties with applications to phosphorescence. Journal of Chemical Physics, 2003, 119, 11024-11034.	3.0	79
84	Linear-scaling implementation of molecular electronic self-consistent field theory. Journal of Chemical Physics, 2007, 126, 114110.	3.0	78
85	Accurate magnetizabilities of the isoelectronic series BeHâº, BH, and CH+. The MCSCF-GIAO approach. Chemical Physics, 1995, 195, 157-169.	1.9	77
86	Accuracy of spectroscopic constants of diatomic molecules from ab initio calculations. Journal of Chemical Physics, 2003, 118, 2539.	3.0	77
87	Variational and robust density fitting of four-center two-electron integrals in local metrics. Journal of Chemical Physics, 2008, 129, 104101.	3.0	75
88	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.	3.0	74
89	A comparison of density-functional-theory and coupled-cluster frequency-dependent polarizabilities and hyperpolarizabilities. Molecular Physics, 2005, 103, 439-450.	1.7	74
90	Magnetizability of Hydrocarbons. Journal of the American Chemical Society, 1994, 116, 10135-10140.	13.7	73

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91	CCSDT calculations of molecular equilibrium geometries. Chemical Physics Letters, 1997, 274, 235-241.	2.6	73
92	Direct optimization of the AO density matrix in Hartreeâ€“Fock and Kohnâ€“Sham theories. Chemical Physics Letters, 2000, 327, 397-403.	2.6	72
93	Coupled-cluster theory for atoms and molecules in strong magnetic fields. Journal of Chemical Physics, 2015, 143, 074110.	3.0	72
94	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.	1.9	71
95	The Molecular Structures of Dimethyl-, Diethyl- and Dipropylzinc Determined by Gas Phase Electron Diffraction. Normal Coordinate Analysis and ab initio Molecular Orbital Calculations on Dimethylzinc.. Acta Chemica Scandinavica, 1982, 36a, 159-166.	0.7	71
96	Electric and magnetic properties of fullerenes. Journal of Chemical Physics, 1998, 109, 572-577.	3.0	70
97	Spinâ€“spin coupling tensors by density-functional linear response theory. Journal of Chemical Physics, 2002, 117, 5998-6009.	3.0	70
98	A gradient extremal walking algorithm. Theoretica Chimica Acta, 1988, 73, 55-65.	0.8	69
99	Gaussian basis sets for high-quality ab initio calculations. The Journal of Physical Chemistry, 1988, 92, 3029-3033.	2.9	69
100	Coupled-cluster connected-quadruples corrections to atomization energies. Chemical Physics Letters, 2003, 371, 62-67.	2.6	68
101	The performance of hybrid density functional theory for the calculation of indirect nuclear spinâ€“spin coupling constants in substituted hydrocarbons. Magnetic Resonance in Chemistry, 2004, 42, S117-S127.	1.9	68
102	Orbital connections for perturbation-dependent basis sets. Theoretica Chimica Acta, 1995, 90, 421-439.	0.8	67
103	The accuracy of molecular dipole moments in standard electronic structure calculations. Chemical Physics Letters, 2000, 319, 563-568.	2.6	67
104	The trust-region self-consistent field method: Towards a black-box optimization in Hartreeâ€“Fock and Kohnâ€“Sham theories. Journal of Chemical Physics, 2004, 121, 16.	3.0	67
105	Attractive electronâ€“electron interactions within robust local fitting approximations. Journal of Computational Chemistry, 2013, 34, 1486-1496.	3.3	67
106	Non-perturbative calculation of molecular magnetic properties within current-density functional theory. Journal of Chemical Physics, 2014, 140, 034101.	3.0	67
107	Ground-state potential energy surface of diazene. Journal of the American Chemical Society, 1987, 109, 2895-2901.	13.7	66
108	Characterization of dihydrogen-bonded Dâ€“Hâ‹¯Hâ€“A complexes on the basis of infrared and magnetic resonance spectroscopic parameters. Journal of Chemical Physics, 2003, 119, 5094-5104.	3.0	66

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109	Current Density Functional Theory Using Meta-Generalized Gradient Exchange-Correlation Functionals. Journal of Chemical Theory and Computation, 2015, 11, 4169-4181.	5.3	66
110	Gauge-origin independent magneto-optical activity within coupled cluster response theory. Journal of Chemical Physics, 2000, 113, 3561-3572.	3.0	64
111	The calculation of adiabatic-connection curves from full configuration-interaction densities: Two-electron systems. Journal of Chemical Physics, 2009, 130, 104111.	3.0	64
112	The NMR indirect nuclear spinâ€“spin coupling constants for some small rigid hydrocarbons: molecular equilibrium values and vibrational corrections. Chemical Physics, 2004, 296, 53-62.	1.9	63
113	Benchmarking density-functional-theory calculations of rotational g tensors and magnetizabilities using accurate coupled-cluster calculations. Journal of Chemical Physics, 2009, 131, 144104.	3.0	60
114	Multiâ€electron integrals. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 290-303.	14.6	60
115	GAUSSIAN BASIS SETS AND MOLECULAR INTEGRALS. Advanced Series in Physical Chemistry, 1995, , 725-856.	1.5	59
116	Rovibrationally averaged magnetizability, rotational g factor, and indirect spinâ€“spin coupling of the hydrogen fluoride molecule. Journal of Chemical Physics, 1999, 110, 9463-9468.	3.0	59
117	Non-perturbative magnetic phenomena in closed-shell paramagnetic molecules. Physical Chemistry Chemical Physics, 2009, 11, 5489.	2.8	59
118	Magnetizability and nuclear shielding constants of solvated water. Chemical Physics Letters, 1996, 253, 443-447.	2.6	58
119	Solvent effects on nuclear shieldings and spinâ€“spin couplings of hydrogen selenide. Journal of Chemical Physics, 1998, 108, 2528-2537.	3.0	58
120	Coupled-cluster singles, doubles and triples (CCSDT) calculations of atomization energies. Chemical Physics Letters, 2000, 317, 116-122.	2.6	58
121	Models of Fragmentations Induced by Electron Attachment to Protonated Peptides. European Journal of Mass Spectrometry, 2004, 10, 625-638.	1.0	58
122	The ab initio calculation of molecular electric, magnetic and geometric properties. Physical Chemistry Chemical Physics, 2011, 13, 2627-2651.	2.8	58
123	A multipole reaction-field model for gauge-origin independent magnetic properties of solvated molecules. Journal of Chemical Physics, 1997, 106, 1170-1180.	3.0	57
124	A Lagrangian, integral-density direct formulation and implementation of the analytic CCSD and CCSD(T) gradients. Journal of Chemical Physics, 2003, 118, 2985-2998.	3.0	57
125	Hartreeâ€“Fock and Kohnâ€“Sham atomic-orbital based time-dependent response theory. Journal of Chemical Physics, 2000, 113, 8908-8917.	3.0	56
126	Spinâ€“spin coupling constants and triplet instabilities in Kohnâ€“Sham theory. Molecular Physics, 2010, 108, 2579-2590.	1.7	55

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127	Choice of exchange-correlation functional for computing NMR indirect spinâ€“spin coupling constants. Chemical Physics Letters, 2006, 425, 163-166.	2.6	54
128	Integral direct calculation of CC2 excitation energies: singlet excited states of benzene. Chemical Physics Letters, 1996, 263, 530-539.	2.6	53
129	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, 2915-2931.	3.0	52
130	Choice of basic variables in current-density-functional theory. Physical Review A, 2012, 86, .	2.5	52
131	Atomic Charges of the Water Molecule and the Water Dimer. Journal of Physical Chemistry A, 1998, 102, 7686-7691.	2.5	51
132	Maps of current density using density-functional methods. Journal of Chemical Physics, 2008, 129, 074101.	3.0	50
133	Calculation of Geometrical Derivatives in Molecular Electronic Structure Theory. NATO ASI Series Series B: Physics, 1992, , 353-421.	0.2	49
134	Frequencyâ€dependent polarizabilities of O2 and van der Waals coefficients of dimers containing O2. Journal of Chemical Physics, 1994, 100, 1297-1302.	3.0	48
135	Differentiable but exact formulation of density-functional theory. Journal of Chemical Physics, 2014, 140, 18A518.	3.0	48
136	Efficient parallel implementation of response theory: Calculations of the second hyperpolarizability of polyacenes. Chemical Physics Letters, 1996, 253, 1-7.	2.6	47
137	Influence of External Force on Properties and Reactivity of Disulfide Bonds. Journal of Physical Chemistry A, 2011, 115, 2308-2315.	2.5	47
138	Spin polarization in restricted electronic structure theory: Multiconfiguration selfâ€consistentâ€field calculations of hyperfine coupling constants. Journal of Chemical Physics, 1992, 97, 3412-3419.	3.0	46
139	Ab initio calculation of electronic circular dichroism fortrans-cyclooctene using London atomic orbitals. Theoretica Chimica Acta, 1995, 90, 441-458.	0.8	46
140	The magnetizability, rotational g tensor, and quadrupole moment of PF3 revisited. Chemical Physics Letters, 1997, 264, 17-23.	2.6	46
141	The effect of correlation on molecular magnetizabilities and rotational g tensors. Journal of Chemical Physics, 1997, 107, 10599-10606.	3.0	45
142	The augmented Roothaanâ€“Hall method for optimizing Hartreeâ€–Fock and Kohnâ€–Sham density matrices. Journal of Chemical Physics, 2008, 129, 124106.	3.0	45
143	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. Journal of Chemical Physics, 2020, 152, 214115.	3.0	45
144	Parity-violating interaction in H2O2 calculated from density-functional theory. Chemical Physics Letters, 2002, 354, 274-282.	2.6	44

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145	Assessment of theoretical methods for the determination of the mechanochemical strength of covalent bonds. Molecular Physics, 2009, 107, 2537-2546.	1.7	44
146	Analytical calculation of MCSCF dipoleâ€moment derivatives. Journal of Chemical Physics, 1986, 84, 6280-6284.	3.0	43
147	Molecular wave functions and properties calculated using floating Gaussian orbitals. Journal of Chemical Physics, 1988, 89, 4889-4902.	3.0	43
148	Density-Functional and Coupled-Cluster Singles-and-Doubles Calculations of the Nuclear Shielding and Indirect Nuclear Spinâ^'Spin Coupling Constants of o-Benzyne. Journal of Chemical Theory and Computation, 2007, 3, 86-94.	5.3	43
149	Analytical GIAO and hybrid-basis integral derivatives: application to geometry optimization of molecules in strong magnetic fields. Physical Chemistry Chemical Physics, 2012, 14, 9492.	2.8	43
150	Second-order MÃ¸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.	1.4	42
151	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.	3.0	42
152	Spin flipping in ring-coupled-cluster-doubles theory. Chemical Physics Letters, 2011, 510, 147-153.	2.6	42
153	Analyzing Magnetically Induced Currents in Molecular Systems Using Current-Density-Functional Theory. Journal of Physical Chemistry A, 2020, 124, 1321-1333.	2.5	42
154	Direct optimization of the atomic-orbital density matrix using the conjugate-gradient method with a multilevel preconditioner. Journal of Chemical Physics, 2001, 115, 9685-9697.	3.0	41
155	Higher molecular-deformation derivatives of the configuration-interaction energy. Chemical Physics, 1984, 86, 413-432.	1.9	40
156	Chemical accuracy from â€˜Coulomb holeâ€™ extrapolated molecular quantum-mechanical calculations. Journal of Molecular Structure, 2001, 567-568, 375-384.	3.6	40
157	Linear-scaling symmetric square-root decomposition of the overlap matrix. Journal of Chemical Physics, 2007, 126, 124104.	3.0	40
158	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.	2.8	40
159	MCSCF calculations of hypermagnetizabilities and nuclear shielding polarizabilities of CO and CH₄. Molecular Physics, 1996, 88, 931-947.	1.7	39
160	The Spinâ€“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.	4.1	39
161	The nuclear spinâ€”spin coupling in N2 and CO. Chemical Physics Letters, 1993, 209, 201-206.	2.6	38
162	Basis-set convergence of the two-electron Darwin term. Chemical Physics Letters, 2000, 319, 287-295.	2.6	38

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163	Computation of two-electron Gaussian integrals for wave functions including the correlation factor r12exp(â^'Î³r122). Computer Physics Communications, 2002, 149, 1-10.	7.5	38
164	Communication: Analytic gradients in the random-phase approximation. Journal of Chemical Physics, 2013, 139, 081101.	3.0	38
165	Analytic cubic and quartic force fields using density-functional theory. Journal of Chemical Physics, 2014, 140, 034103.	3.0	38
166	Fractional Electron Loss in Approximate DFT and Hartreeâ€"Fock Theory. Journal of Chemical Theory and Computation, 2015, 11, 5262-5268.	5.3	38
167	The Calculation of Indirect Nuclear Spin-Spin Coupling Constants in Large Molecules. Chemistry - A European Journal, 2004, 10, 4627-4639.	3.3	37
168	Implementation of the incremental scheme for one-electron first-order properties in coupled-cluster theory. Journal of Chemical Physics, 2009, 131, 154102.	3.0	37
169	Alternative separation of exchange and correlation energies in multi-configuration range-separated density-functional theory. Journal of Chemical Physics, 2013, 139, 134113.	3.0	37
170	On the evaluation of derivatives of Gaussian integrals. Theoretica Chimica Acta, 1992, 83, 177-183.	0.8	36
171	Geometrical derivatives and magnetic properties in atomic-orbital density-based Hartreeâ€"Fock theory. Journal of Chemical Physics, 2001, 115, 10344.	3.0	36
172	NMR Shielding Tensors and Indirect Spin-Spin Coupling Tensors in HCN, HNC, CH3CN, and Ch3NC Molecules. Journal of Magnetic Resonance Series A, 1995, 114, 212-218.	1.6	35
173	Efficient elimination of response parameters in molecular property calculations for variational and nonvariational energies. Journal of Chemical Physics, 2008, 129, 214103.	3.0	35
174	The importance of current contributions to shielding constants in density-functional theory. Physical Chemistry Chemical Physics, 2015, 17, 18834-18842.	2.8	35
175	Solvent effects on the NMR parameters of H2S and HCN. Journal of Computational Chemistry, 1999, 20, 1281-1291.	3.3	34
176	Interconversion of diborane (4) isomers. Journal of Chemical Physics, 1992, 97, 1211-1216.	3.0	33
177	Accurate molecular geometries of the protonated water dimer. Physical Chemistry Chemical Physics, 2000, 2, 2235-2238.	2.8	33
178	A unified scheme for the calculation of differentiated and undifferentiated molecular integrals over solid-harmonic Gaussians. Physical Chemistry Chemical Physics, 2007, 9, 4771.	2.8	33
179	Orbital connections for perturbation-dependent basis sets. Theoretica Chimica Acta, 1995, 90, 421.	0.8	33
180	Basis set convergence and correlation effects in vibrational circular dichroism calculations using London atomic orbitals. Faraday Discussions, 1994, 99, 121-129.	3.2	32

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181	Energetics and Dynamics of Intermolecular Proton-Transfer Processes. 2. Ab Initio Direct Dynamics Calculations of the Reaction H3O++ NH3â† NH4++ H2O. The Journal of Physical Chemistry, 1996, 100, 15388-15392.	2.9	32
182	Magnetizabilities and Nuclear Shielding Constants of the Fluoromethanes in the Gas Phase and Solution. The Journal of Physical Chemistry, 1996, 100, 19771-19782.	2.9	32
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