Trygve Helgaker

List of Publications by Year in descending order

348 papers	31,566 citations	7251 80 h-index	6512 162 g-index
371 all docs	371 docs citations	371 times ranked	13517 citing authors

#	Article	IF	Citations
1	Analytic calculation of the Berry curvature and diagonal Bornâ€“Oppenheimer correction for molecular systems in uniform magnetic fields. Journal of Chemical Physics, 2022, 156, 044121.	1.2	15
2	Revealing the exotic structure of molecules in strong magnetic fields. Journal of Chemical Physics, 2022, 156, .	1.2	11
3	Molecular dynamics of linear molecules in strong magnetic fields. Journal of Chemical Physics, 2022, 157, .	1.2	13
4	Lower Semicontinuity of the Universal Functional in Paramagnetic Currentâ€“Density Functional Theory. Journal of Physical Chemistry Letters, 2021, 12, 1421-1425.	2.1	11
5	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.	1.2	16
6	Ab initio molecular dynamics with screened Lorentz forces. I. Calculation and atomic charge interpretation of Berry curvature. Journal of Chemical Physics, 2021, 155, 024104.	1.2	23
7	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.	1.1	8
8	Bonding in the helium dimer in strong magnetic fields: the role of spin and angular momentum. Physical Chemistry Chemical Physics, 2020, 22, 23502-23521.	1.3	15
9	Foreword: Prof. Gauss Festschrift. Molecular Physics, 2020, 118, e1817247.	0.8	0
10	Analyzing Magnetically Induced Currents in Molecular Systems Using Current-Density-Functional Theory. Journal of Physical Chemistry A, 2020, 124, 1321-1333.	1.1	42
11	Challenges for large scale simulation: general discussion. Faraday Discussions, 2020, 224, 309-332.	1.6	2
12	New density-functional approximations and beyond: general discussion. Faraday Discussions, 2020, 224, 166-200.	1.6	1
13	First-Principles Calculation of ¹H NMR Chemical Shifts of Complex Metal Polyhydrides: The Essential Inclusion of Relativity and Dynamics. Inorganic Chemistry, 2020, 59, 17509-17518.	1.9	12
14	Strong correlation in density functional theory: general discussion. Faraday Discussions, 2020, 224, 373-381.	1.6	2
15	New approaches to study excited states in density functional theory: general discussion. Faraday Discussions, 2020, 224, 483-508.	1.6	2
16	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. Journal of Chemical Physics, 2020, 152, 214115.	1.2	45
17	Atoms and molecules in soft confinement potentials. Molecular Physics, 2020, 118, e1730989.	0.8	18
18	A quantum-mechanical non-Bornâ€“Oppenheimer model of a molecule in a strong magnetic field. Chemical Physics Letters, 2020, 761, 138041.	1.2	4

#	Article	IF	Citations
19	Kohnâ€“Sham energy decomposition for molecules in a magnetic field. Molecular Physics, 2019, 117, 97-109.	0.8	21
20	GW quasiparticle energies of atoms in strong magnetic fields. Journal of Chemical Physics, 2019, 150, 214112.	1.2	21
21	Kohnâ€“Sham Theory with Paramagnetic Currents: Compatibility and Functional Differentiability. Journal of Chemical Theory and Computation, 2019, 15, 4003-4020.	2.3	14
22	Four-component relativistic ³¹P NMR calculations for trans-platinum(<scp>ii</scp>) complexes: importance of the solvent and dynamics in spectral simulations. Dalton Transactions, 2019, 48, 8076-8083.	1.6	18
23	Excitation energies from GÃ¶rlingâ€“Levy perturbation theory along the range-separated adiabatic connection. Molecular Physics, 2018, 116, 1443-1451.	0.8	5
24	Uniform magnetic fields in density-functional theory. Journal of Chemical Physics, 2018, 148, 024101.	1.2	20
25	A computational quantum-mechanical model of a molecular magnetic trap. Journal of Chemical Physics, 2018, 149, 244112.	1.2	6
26	Betheâ€“Salpeter correlation energies of atoms and molecules. Journal of Chemical Physics, 2018, 149, 144106.	1.2	24
27	Generalized Kohnâ€“Sham iteration on Banach spaces. Journal of Chemical Physics, 2018, 149, 164103.	1.2	14
28	Explicitly-correlated non-born-oppenheimer calculations of the HD molecule in a strong magnetic field. Chemical Physics Letters, 2017, 682, 87-90.	1.2	7
29	Connections between variation principles at the interface of wave-function and density-functional theories. Journal of Chemical Physics, 2017, 147, 134107.	1.2	4
30	Magnetic-Field Density-Functional Theory (BDFT): Lessons from the Adiabatic Connection. Journal of Chemical Theory and Computation, 2017, 13, 4089-4100.	2.3	32
31	A tribute to Jan Erik AlmlÃ¶f. Molecular Physics, 2017, 115, 2033-2042.	0.8	0
32	Nuclei-selected atomic-orbital response-theory formulation for the calculation of NMR shielding tensors using density-fitting. Journal of Chemical Physics, 2016, 145, 234108.	1.2	7
33	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, 3514-3522.	2.3	29
34	Calculation of NMR Spinâ€“Spin Coupling Constants in Strychnine. Journal of Organic Chemistry, 2016, 81, 11496-11500.	1.7	20
35	Foreword for special issue of Molecular Physics in honour of Andreas Savin. Molecular Physics, 2016, 114, 909-909.	0.8	0
36	Alternative Representations of the Correlation Energy in Densityâ€Functional Theory: A Kineticâ€Energy Based Adiabatic Connection. Journal of the Chinese Chemical Society, 2016, 63, 121-128.	0.8	7

#	Article	IF	Citations
37	Electron localisation function in current-density-functional theory. Molecular Physics, 2016, 114, 1415-1422.	0.8	14
38	Coupled-cluster theory for atoms and molecules in strong magnetic fields. Journal of Chemical Physics, 2015, 143, 074110.	1.2	72
39	Ground-state densities from the Rayleighâ€“Ritz variation principle and from density-functional theory. Journal of Chemical Physics, 2015, 143, 184106.	1.2	11
40	FemExâ€”female excellence in theoretical and computational chemistry. International Journal of Quantum Chemistry, 2015, 115, 1195-1196.	1.0	3
41	Excited states from range-separated density-functional perturbation theory. Molecular Physics, 2015, 113, 1740-1749.	0.8	12
42	Geometry of the magic number H⁺(H₂O)₂₁water cluster by proxy. Physical Chemistry Chemical Physics, 2015, 17, 5466-5473.	1.3	9
43	Use of Density Functional Theory Orbitals in the GVVPT2 Variant of Second-Order Multistate Multireference Perturbation Theory. Journal of Physical Chemistry A, 2015, 119, 1548-1553.	1.1	9
44	Current Density Functional Theory Using Meta-Generalized Gradient Exchange-Correlation Functionals. Journal of Chemical Theory and Computation, 2015, 11, 4169-4181.	2.3	66
45	The importance of current contributions to shielding constants in density-functional theory. Physical Chemistry Chemical Physics, 2015, 17, 18834-18842.	1.3	35
46	Calculating excitation energies by extrapolation along adiabatic connections. Physical Review A, 2015, 91, .	1.0	14
47	Molecular properties in the Tammâ€“Dancoff approximation: indirect nuclear spinâ€“spin coupling constants. Molecular Physics, 2015, 113, 1937-1951.	0.8	9
48	Fractional Electron Loss in Approximate DFT and Hartreeâ€“Fock Theory. Journal of Chemical Theory and Computation, 2015, 11, 5262-5268.	2.3	38
49	Non-Bornâ€“Oppenheimer calculations of the HD molecule in a strong magnetic field. Chemical Physics Letters, 2015, 639, 295-299.	1.2	10
50	Excitation energies from ensemble DFT. AIP Conference Proceedings, 2015, , .	0.3	2
51	Non-perturbative calculation of molecular magnetic properties within current-density functional theory. Journal of Chemical Physics, 2014, 140, 034101.	1.2	67
52	Fermion<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>N</mml:mi></mml:math>-representability for prescribed density and paramagnetic current density. Physical Review A, 2014, 89, .	1.0	14
53	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	6.2	1,166
54	Excitation energies along a range-separated adiabatic connection. Journal of Chemical Physics, 2014, 141, 044123.	1.2	17

#	Article	IF	Citations
55	Charge-constrained auxiliary-density-matrix methods for the Hartreeâ€“Fock exchange contribution. Journal of Chemical Physics, 2014, 141, 094104.	1.2	21
56	Analytic cubic and quartic force fields using density-functional theory. Journal of Chemical Physics, 2014, 140, 034103.	1.2	38
57	Mechanochemistry: The Effect of Dynamics. Journal of Physical Chemistry A, 2014, 118, 7683-7694.	1.1	22
58	Differentiable but exact formulation of density-functional theory. Journal of Chemical Physics, 2014, 140, 18A518.	1.2	48
59	Multiconfigurational Self-Consistent Field Theory. , 2014, , 598-647.		4
60	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.	1.0	5
61	Communication: Analytic gradients in the random-phase approximation. Journal of Chemical Physics, 2013, 139, 081101.	1.2	38
62	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.	1.2	153
63	Attractive electronâ€“electron interactions within robust local fitting approximations. Journal of Computational Chemistry, 2013, 34, 1486-1496.	1.5	67
64	Internalâ€toâ€Cartesian back transformation of molecular geometry steps using highâ€order geometric derivatives. Journal of Computational Chemistry, 2013, 34, 1842-1849.	1.5	6
65	The accuracy of the Gaussian-and-finite-element-Coulomb (GFC) method for the calculation of Coulomb integrals. Journal of Chemical Physics, 2013, 139, 054114.	1.2	2
66	33S hyperfine interactions in H2S and SO2 and revision of the sulfur nuclear magnetic shielding scale. Journal of Chemical Physics, 2013, 139, 244308.	1.2	22
67	Insights into the dynamics of evaporation and proton migration in protonated water clusters from Largeâ€scale Bornâ€“Oppenheimer direct dynamics. Journal of Computational Chemistry, 2013, 34, 533-544.	1.5	7
68	Alternative separation of exchange and correlation energies in multi-configuration range-separated density-functional theory. Journal of Chemical Physics, 2013, 139, 134113.	1.2	37
69	A Theoretical Study on Proton Conduction Mechanism in BaZrO3 Perovskite. Progress in Theoretical Chemistry and Physics, 2013, , 233-248.	0.2	8
70	Choice of basic variables in current-density-functional theory. Physical Review A, 2012, 86, .	1.0	52
71	The NMR indirect nuclear spinâ€“spin coupling constant of the HD molecule. Molecular Physics, 2012, 110, 2611-2617.	0.8	15
72	Analytical GIAO and hybrid-basis integral derivatives: application to geometry optimization of molecules in strong magnetic fields. Physical Chemistry Chemical Physics, 2012, 14, 9492.	1.3	43

#	Article	IF	Citations
73	A Paramagnetic Bonding Mechanism for Diatomics in Strong Magnetic Fields. Science, 2012, 337, 327-331.	6.0	123
74	Range-dependent adiabatic connections. , 2012, , .		0
75	A theoretical study on hydrogen transport mechanism in SrTio₃ perovskite. International Journal of Quantum Chemistry, 2012, 112, 201-207.	1.0	8
76	Multiâ€electron integrals. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 290-303.	6.2	60
77	Recent Advances in Wave Function-Based Methods of Molecular-Property Calculations. Chemical Reviews, 2012, 112, 543-631.	23.0	549
78	Calculation of the two-electron Darwin term using explicitly correlated wave functions. Chemical Physics, 2012, 401, 146-151.	0.9	3
79	Influence of External Force on Properties and Reactivity of Disulfide Bonds. Journal of Physical Chemistry A, 2011, 115, 2308-2315.	1.1	47
80	Dispersion interactions in density-functional theory: An adiabatic-connection analysis. Journal of Chemical Physics, 2011, 135, 194109.	1.2	21
81	The ab initio calculation of molecular electric, magnetic and geometric properties. Physical Chemistry Chemical Physics, 2011, 13, 2627-2651.	1.3	58
82	Relativistic four-component calculations of Buckingham birefringence using London atomic orbitals. Theoretical Chemistry Accounts, 2011, 129, 685-699.	0.5	4
83	Spin flipping in ring-coupled-cluster-doubles theory. Chemical Physics Letters, 2011, 510, 147-153.	1.2	42
84	Range-dependent adiabatic connections. Journal of Chemical Physics, 2010, 133, 164112.	1.2	30
85	An efficient density-functional-theory force evaluation for large molecular systems. Journal of Chemical Physics, 2010, 133, 044102.	1.2	20
86	Accurate calculation and modeling of the adiabatic connection in density functional theory. Journal of Chemical Physics, 2010, 132, 164115.	1.2	86
87	Spinâ€“spin coupling constants and triplet instabilities in Kohnâ€“Sham theory. Molecular Physics, 2010, 108, 2579-2590.	0.8	55
88	Benchmarking density-functional-theory calculations of rotational g tensors and magnetizabilities using accurate coupled-cluster calculations. Journal of Chemical Physics, 2009, 131, 144104.	1.2	60
89	Implementation of the incremental scheme for one-electron first-order properties in coupled-cluster theory. Journal of Chemical Physics, 2009, 131, 154102.	1.2	37
90	The geminal basis in explicitly correlated wave functions. Chemical Physics, 2009, 356, 25-30.	0.9	24

#	Article	IF	Citations
91	Robust and Reliable Multilevel Minimization of the Kohnâ^'Sham Energy. Journal of Chemical Theory and Computation, 2009, 5, 1027-1032.	2.3	12
92	The calculation of adiabatic-connection curves from full configuration-interaction densities: Two-electron systems. Journal of Chemical Physics, 2009, 130, 104111.	1.2	64
93	Assessment of theoretical methods for the determination of the mechanochemical strength of covalent bonds. Molecular Physics, 2009, 107, 2537-2546.	0.8	44
94	Non-perturbative magnetic phenomena in closed-shell paramagnetic molecules. Physical Chemistry Chemical Physics, 2009, 11, 5489.	1.3	59
95	A stepwise atomic, valence-molecular, and full-molecular optimisation of the Hartreeâ€"Fock/Kohnâ€"Sham energy. Physical Chemistry Chemical Physics, 2009, 11, 5805.	1.3	15
96	The quantum-chemical calculation of NMR indirect spinâ€"spin coupling constants. Progress in Nuclear Magnetic Resonance Spectroscopy, 2008, 53, 249-268.	3.9	252
97	Static and Frequencyâ€Dependent Dipoleâ€"Dipole Polarizabilities of All Closedâ€Shell Atoms up to Radium: A Fourâ€Component Relativistic DFT Study. ChemPhysChem, 2008, 9, 445-453.	1.0	27
98	Excitation energies in density functional theory: An evaluation and a diagnostic test. Journal of Chemical Physics, 2008, 128, 044118.	1.2	1,190
99	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.	1.2	42
100	Maps of current density using density-functional methods. Journal of Chemical Physics, 2008, 129, 074101.	1.2	50
101	Quantitative quantum chemistry. Molecular Physics, 2008, 106, 2107-2143.	0.8	215
102	Variational and robust density fitting of four-center two-electron integrals in local metrics. Journal of Chemical Physics, 2008, 129, 104101.	1.2	75
103	A ground-state-directed optimization scheme for the Kohnâ€"Sham energy. Physical Chemistry Chemical Physics, 2008, 10, 5344.	1.3	16
104	Second-order MÃ¸llerâ€"Plesset calculations on the water molecule using Gaussian-type orbital and Gaussian-type geminal theory. Physical Chemistry Chemical Physics, 2008, 10, 3377.	1.3	13
105	Nonperturbative ab initio calculations in strong magnetic fields using London orbitals. Journal of Chemical Physics, 2008, 129, 154114.	1.2	99
106	Efficient elimination of response parameters in molecular property calculations for variational and nonvariational energies. Journal of Chemical Physics, 2008, 129, 214103.	1.2	35
107	Density-functional calculations of the nuclear magnetic shielding and indirect nuclear spinâ€"spin coupling constants of three isomers of C20. Molecular Physics, 2008, 106, 2357-2365.	0.8	3
108	The augmented Roothaanâ€"Hall method for optimizing Hartreeâ€"Fock and Kohnâ€"Sham density matrices. Journal of Chemical Physics, 2008, 129, 124106.	1.2	45

#	Article	IF	Citations
109	Electronic circular dichroism of disulphide bridge: Ab initio quantum-chemical calculations. Journal of Chemical Physics, 2007, 127, 085102.	1.2	18
110	Linear-scaling implementation of molecular electronic self-consistent field theory. Journal of Chemical Physics, 2007, 126, 114110.	1.2	78
111	Linear-scaling implementation of molecular response theory in self-consistent field electronic-structure theory. Journal of Chemical Physics, 2007, 126, 154108.	1.2	87
112	A unified scheme for the calculation of differentiated and undifferentiated molecular integrals over solid-harmonic Gaussians. Physical Chemistry Chemical Physics, 2007, 9, 4771.	1.3	33
113	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.	2.3	43
114	Linear-scaling symmetric square-root decomposition of the overlap matrix. Journal of Chemical Physics, 2007, 126, 124104.	1.2	40
115	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.	1.3	40
116	Structural and Electronic Properties of Polyacetylene and Polyyne from Hybrid and Coulomb-Attenuated Density Functionals. Journal of Physical Chemistry A, 2007, 111, 11930-11935.	1.1	139
117	Explicit Electron Correlation by a Combined Use of Gaussian-Type Orbitals and Gaussian-Type Geminals. AIP Conference Proceedings, 2007, , .	0.3	0
118	Electron correlation: The many-body problem at the heart of chemistry. Journal of Computational Chemistry, 2007, 28, 1307-1320.	1.5	82
119	Assessment of a Coulomb-attenuated exchangeâ€"correlation energy functional. Physical Chemistry Chemical Physics, 2006, 8, 558-562.	1.3	437
120	RotationalgTensors Calculated Using Hybrid Exchange-Correlation Functionals with the Optimized Effective Potential Approach. Journal of Chemical Theory and Computation, 2006, 2, 827-834.	2.3	14
121	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.	1.2	99
122	Choice of exchange-correlation functional for computing NMR indirect spinâ€"spin coupling constants. Chemical Physics Letters, 2006, 425, 163-166.	1.2	54
123	The Equilibrium Structure of Ferrocene. ChemPhysChem, 2006, 7, 245-249.	1.0	149
124	A second-quantization framework for the unified treatment of relativistic and nonrelativistic molecular perturbations by response theory. Journal of Chemical Physics, 2006, 125, 024102.	1.2	6
125	Benchmarking two-photon absorption with CC3 quadratic response theory, and comparison with density-functional response theory. Journal of Chemical Physics, 2006, 124, 054322.	1.2	137
126	The magnetizability, rotational g tensor and quadrupole moment of the boron trihalides. Molecular Physics, 2006, 104, 847-856.	0.8	4

#	Article	IF	Citations
127	Self-consistent field methods applied to large molecular systems. , 2006, , 1297-1297.		0
128	Towards black-box linear scaling optimization in Hartree-Fock and Kohn-Sham theories. , 2006, , 177-189.		0
129	The Rotational g Tensor as a Benchmark for Ab Initio Molecular Property Calculations. Advances in Quantum Chemistry, 2005, , 77-90.	0.4	5
130	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.	0.9	71
131	The accuracy ofab initiomolecular geometries for systems containing second-row atoms. Journal of Chemical Physics, 2005, 123, 184107.	1.2	125
132	A computational study of some electric and magnetic properties of gaseous BF3 and BCl3. Journal of Chemical Physics, 2005, 123, 114307.	1.2	9
133	The trust-region self-consistent field method in Kohnâ€“Sham density-functional theory. Journal of Chemical Physics, 2005, 123, 074103.	1.2	31
134	Density-functional theory study of electric and magnetic properties of hexafluorobenzene in the vapor phase. Journal of Chemical Physics, 2005, 122, 234314.	1.2	27
135	Calculations of two-photon charge-transfer excitations using Coulomb-attenuated density-functional theory. Journal of Chemical Physics, 2005, 123, 184108.	1.2	112
136	A comparison of density-functional-theory and coupled-cluster frequency-dependent polarizabilities and hyperpolarizabilities. Molecular Physics, 2005, 103, 439-450.	0.8	74
137	Theoretical Studies of Nuclear Magnetic Resonance Parameters for the Proton-Exchange Pathways in Porphyrin and Porphycene. Journal of Physical Chemistry A, 2005, 109, 4162-4171.	1.1	22
138	The RotationalgTensor as a Benchmark for Density-Functional Theory Calculations of Molecular Magnetic Properties. Journal of Chemical Theory and Computation, 2005, 1, 877-888.	2.3	30
139	Atmospheric Chemistry of CHF2CHO:Â Study of the IR and UVâ"Vis Absorption Cross Sections, Photolysis, and OH-, Cl-, and NO3-Initiated Oxidation. Journal of Physical Chemistry A, 2005, 109, 3652-3662.	1.1	7
140	Quadratic Response Functions in a Second-Order Polarization Propagator Frameworkâ€. Journal of Physical Chemistry A, 2005, 109, 11618-11628.	1.1	29
141	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.	0.6	21
142	A closed-shell coupled-cluster treatment of the Breitâ€“Pauli first-order relativistic energy correction. Journal of Chemical Physics, 2004, 121, 6591-6598.	1.2	29
143	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.	1.2	125
144	Calculation of electric dipole hypershieldings at the nuclei in the Hellmannâ€“Feynman approximation. Journal of Chemical Physics, 2004, 120, 3142-3151.	1.2	11

#	Article	IF	Citations
145	Polarization consistent basis sets. V. The elements Siâ€“Cl. Journal of Chemical Physics, 2004, 121, 3463-3470.	1.2	181
146	The expansion of hydrogen states in Gaussian orbitals. Theoretical Chemistry Accounts, 2004, 112, 124.	0.5	4
147	A priori calculation of molecular properties to chemical accuracy. Journal of Physical Organic Chemistry, 2004, 17, 913-933.	0.9	204
148	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.	1.1	68
149	The Calculation of Indirect Nuclear Spin-Spin Coupling Constants in Large Molecules. Chemistry - A European Journal, 2004, 10, 4627-4639.	1.7	37
150	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.	0.9	63
151	Density functional theory calculation of electronic circular dichroism using London orbitals. Chemical Physics Letters, 2004, 388, 110-119.	1.2	123
152	GIAO shielding constants and indirect spinâ€“spin coupling constants: performance of density functional methods. Chemical Physics Letters, 2004, 391, 374-379.	1.2	87
153	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.	1.2	67
154	Conformational Effects on the Optical Rotation of Alanine and Proline. Journal of Physical Chemistry A, 2004, 108, 4269-4276.	1.1	103
155	Density-functional theory calculations of optical rotatory dispersion in the nonresonant and resonant frequency regions. Journal of Chemical Physics, 2004, 120, 5027-5035.	1.2	81
156	Potential Energy and Spinâˆ'Spin Coupling Constants Surface of Glycolaldehyde. Journal of Physical Chemistry A, 2004, 108, 2758-2769.	1.1	18
157	A comparison of polarization and bond functions for density functional calculations. Molecular Physics, 2004, 102, 2559-2562.	0.8	3
158	Spin-Spin Coupling Constants with HF and DFT Methods. , 2004, , 101-121.		25
159	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.	1.2	52
160	Density-functional generalized-gradient and hybrid calculations of electromagnetic properties using Slater basis sets. Journal of Chemical Physics, 2004, 120, 7252-7261.	1.2	28
161	Models of Fragmentations Induced by Electron Attachment to Protonated Peptides. European Journal of Mass Spectrometry, 2004, 10, 625-638.	0.5	58
162	Coupled-cluster connected-quadruples corrections to atomization energies. Chemical Physics Letters, 2003, 371, 62-67.	1.2	68

#	Article	IF	Citations
163	Sternheimer shieldings and EFG polarizabilities: a density-functional theory study. Chemical Physics Letters, 2003, 372, 377-385.	1.2	4
164	Calculations of hydrogen-bond-transmitted indirect nuclear spinâ€“spin couplings: a comparison of density-functional and ab initio methods. Chemical Physics Letters, 2003, 372, 476-484.	1.2	27
165	Calculations of two-photon absorption cross sections by means of density-functional theory. Chemical Physics Letters, 2003, 374, 446-452.	1.2	136
166	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.	1.2	66
167	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.	1.8	39
168	Density-functional theory calculation of the nuclear magnetic resonance indirect nuclear spinâ€”spin coupling constants in C60. Molecular Physics, 2003, 101, 1997-2002.	0.8	18
169	Density functional theory of nonlinear triplet response properties with applications to phosphorescence. Journal of Chemical Physics, 2003, 119, 11024-11034.	1.2	79
170	Accuracy of spectroscopic constants of diatomic molecules from ab initio calculations. Journal of Chemical Physics, 2003, 118, 2539.	1.2	77
171	A Lagrangian, integral-density direct formulation and implementation of the analytic CCSD and CCSD(T) gradients. Journal of Chemical Physics, 2003, 118, 2985-2998.	1.2	57
172	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.	1.2	74
173	Vibrational corrections to indirect nuclear spinâ€“spin coupling constants calculated by density-functional theory. Journal of Chemical Physics, 2003, 118, 9572-9581.	1.2	156
174	Wave Functionâ€“Based Quantum Chemistry. , 2003, , .		0
175	Vibronic transitions from coupled-cluster response theory: Theory and application to HSiF and H[sub 2]O. Journal of Chemical Physics, 2002, 116, 8334.	1.2	8
176	Molecular equilibrium structures from experimental rotational constants and calculated vibrationâ€“rotation interaction constants. Journal of Chemical Physics, 2002, 116, 6482-6496.	1.2	245
177	Gauge-Origin Independent Density-Functional Theory Calculations of Vibrational Raman Optical Activity. Journal of Physical Chemistry A, 2002, 106, 7448-7455.	1.1	162
178	The efficient optimization of molecular geometries using redundant internal coordinates. Journal of Chemical Physics, 2002, 117, 9160-9174.	1.2	109
179	Spinâ€“spin coupling tensors by density-functional linear response theory. Journal of Chemical Physics, 2002, 117, 5998-6009.	1.2	70
180	Density-functional theory of linear and nonlinear time-dependent molecular properties. Journal of Chemical Physics, 2002, 117, 9630-9645.	1.2	359

#	Article	IF	Citations
181	Four-component relativistic Kohn-Sham theory. Journal of Computational Chemistry, 2002, 23, 814-823.	1.5	147
182	Basis-set completeness profiles in two dimensions. Journal of Computational Chemistry, 2002, 23, 420-425.	1.5	9
183	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.	0.5	42
184	Computation of two-electron Gaussian integrals for wave functions including the correlation factor r12exp(â^'Î³r122). Computer Physics Communications, 2002, 149, 1-10.	3.0	38
185	Optical rotation studied by density-functional and coupled-cluster methods. Chemical Physics Letters, 2002, 352, 533-539.	1.2	192
186	Parity-violating interaction in H2O2 calculated from density-functional theory. Chemical Physics Letters, 2002, 354, 274-282.	1.2	44
187	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.	1.2	41
188	Efficient evaluation of one-center three-electron Gaussian integrals. Theoretical Chemistry Accounts, 2001, 106, 280-286.	0.5	18
189	Chemical accuracy from â€˜Coulomb holeâ€™ extrapolated molecular quantum-mechanical calculations. Journal of Molecular Structure, 2001, 567-568, 375-384.	1.8	40
190	Geometrical derivatives and magnetic properties in atomic-orbital density-based Hartreeâ€“Fock theory. Journal of Chemical Physics, 2001, 115, 10344.	1.2	36
191	Direct perturbation theory of magnetic properties and relativistic corrections for the point nuclear and Gaussian nuclear models. Journal of Chemical Physics, 2001, 115, 7356-7363.	1.2	32
192	The accurate determination of molecular equilibrium structures. Journal of Chemical Physics, 2001, 114, 6548-6556.	1.2	353
193	Highly Accurate Ab Initio Computation of Thermochemical Data. , 2001, , 1-30.		4
194	Basis-set convergence of the two-electron Darwin term. Chemical Physics Letters, 2000, 319, 287-295.	1.2	38
195	The accuracy of molecular dipole moments in standard electronic structure calculations. Chemical Physics Letters, 2000, 319, 563-568.	1.2	67
196	Direct optimization of the AO density matrix in Hartreeâ€“Fock and Kohnâ€“Sham theories. Chemical Physics Letters, 2000, 327, 397-403.	1.2	72
197	Coupled-cluster singles, doubles and triples (CCSDT) calculations of atomization energies. Chemical Physics Letters, 2000, 317, 116-122.	1.2	58
198	Perspective on "Neue Berechnung der Energie des Heliums im Grundzustande, sowie des tiefsten Terms von Ortho-Helium". Theoretical Chemistry Accounts, 2000, 103, 180-181.	0.5	9

#	Article	IF	Citations
199	Nuclear shielding constants by density functional theory with gauge including atomic orbitals. Journal of Chemical Physics, 2000, 113, 2983-2989.	1.2	104
200	Divergence in MÃ¸llerâ€“Plesset theory: A simple explanation based on a two-state model. Journal of Chemical Physics, 2000, 112, 9736-9748.	1.2	79
201	Gauge-origin independent magneto-optical activity within coupled cluster response theory. Journal of Chemical Physics, 2000, 113, 3561-3572.	1.2	64
202	Hartreeâ€“Fock and Kohnâ€“Sham atomic-orbital based time-dependent response theory. Journal of Chemical Physics, 2000, 113, 8908-8917.	1.2	56
203	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.	1.2	345
204	Should Gaseous BF3 and SiF4 Be Described as Ionic Compounds?. Journal of Chemical Education, 2000, 77, 1076.	1.1	24
205	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.	1.2	224
206	Accurate molecular geometries of the protonated water dimer. Physical Chemistry Chemical Physics, 2000, 2, 2235-2238.	1.3	33
207	Perspective on â€œNeue Berechnung der Energie des Heliums im Grundzustande, sowie des tiefsten Terms von Ortho-Heliumâ€•, 2000, 103, 180.		2
208	Molecular polarizabilities and magnetizabilities. Theoretical and Computational Chemistry, 1999, , 147-188.	0.2	3
209	Rovibrationally averaged magnetizability, rotational g factor, and indirect spinâ€“spin coupling of the hydrogen fluoride molecule. Journal of Chemical Physics, 1999, 110, 9463-9468.	1.2	59
210	Basis-set convergence of the energy in molecular Hartreeâ€“Fock calculations. Chemical Physics Letters, 1999, 302, 437-446.	1.2	604
211	Solvent effects on the NMR parameters of H2S and HCN. , 1999, 20, 1281-1291.		34
212	Basis-set convergence of the molecular electric dipole moment. Journal of Chemical Physics, 1999, 111, 4424-4430.	1.2	114
213	Highly accurate calculations of molecular electronic structure. Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, R103-R130.	0.6	214
214	The calculation of molecular geometrical properties in the Hellmannâ€”Feynman approximation. Molecular Physics, 1999, 96, 653-671.	0.8	12
215	Basis set convergence of the interaction energy of hydrogen-bonded complexes. Journal of Chemical Physics, 1999, 111, 9157-9167.	1.2	363
216	Ab Initio Methods for the Calculation of NMR Shielding and Indirect Spinâˆ’Spin Coupling Constants. Chemical Reviews, 1999, 99, 293-352.	23.0	1,318

#	Article	IF	Citations
217	The calculation of molecular geometrical properties in the Hellmann-Feynman approximation. Molecular Physics, 1999, 96, 653-671.	0.8	21
218	The Hartreeâ€“Fock magnetizability of C60. Chemical Physics Letters, 1998, 285, 205-209.	1.2	16
219	Basis-set convergence in correlated calculations on Ne, N2, and H2O. Chemical Physics Letters, 1998, 286, 243-252.	1.2	1,989
220	Vibrationally averaged magnetizabilities and rotational g tensors of the water molecule. Chemical Physics Letters, 1998, 297, 467-474.	1.2	25
221	Spin-orbit and correlation effects in platinum hydride (PtH). International Journal of Quantum Chemistry, 1998, 68, 53-64.	1.0	10
222	Basis-set dependence of nuclear spin-spin coupling constants. Theoretical Chemistry Accounts, 1998, 99, 175-182.	0.5	175
223	Extrapolation to the limit of a complete basis set for electronic structure calculations on the N 2 molecule. Theoretical Chemistry Accounts, 1998, 99, 265-271.	0.5	30
224	Atomic Charges of the Water Molecule and the Water Dimer. Journal of Physical Chemistry A, 1998, 102, 7686-7691.	1.1	51
225	Solvent effects on nuclear shieldings and spinâ€“spin couplings of hydrogen selenide. Journal of Chemical Physics, 1998, 108, 2528-2537.	1.2	58
226	Electric and magnetic properties of fullerenes. Journal of Chemical Physics, 1998, 109, 572-577.	1.2	70
227	Electric field gradient, generalized Sternheimer shieldings and electric field gradient polarizabilities by multiconfigurational SCF response. Journal of Chemical Physics, 1998, 109, 2264-2274.	1.2	14
228	Integral-direct coupled cluster calculations of frequency-dependent polarizabilities, transition probabilities and excited-state properties. Journal of Chemical Physics, 1998, 108, 2801-2816.	1.2	191
229	The Cottonâ€“Mouton effect of liquid water. Part II: The semi-continuum model. Journal of Chemical Physics, 1998, 108, 599-603.	1.2	20
230	Generalized integral-screening for efficient calculations of nonlinear optical properties of large molecules. Journal of Chemical Physics, 1998, 108, 7973-7979.	1.2	16
231	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.	1.2	115
232	The Molecular Zeeman Effect of Norbornadiene, its g-Values, Magnetizability Anisotropics, and Molecular Electric Quadrupole Moment; A High-Resolution Microwave Fourier-Transform Study Combined with Quantum Chemical Calculations. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1998, 53, 67-76.	0.7	3
233	Electric and magnetic properties of the nitroethene molecule. Molecular Physics, 1997, 92, 89-96.	0.8	11
234	The effect of correlation on molecular magnetizabilities and rotational g tensors. Journal of Chemical Physics, 1997, 107, 10599-10606.	1.2	45

#	Article	IF	Citations
235	A multipole reaction-field model for gauge-origin independent magnetic properties of solvated molecules. Journal of Chemical Physics, 1997, 106, 1170-1180.	1.2	57
236	The CC3 model: An iterative coupled cluster approach including connected triples. Journal of Chemical Physics, 1997, 106, 1808-1818.	1.2	412
237	First-order one-electron properties in the integral-direct coupled cluster singles and doubles model. Journal of Chemical Physics, 1997, 107, 849-866.	1.2	122
238	The prediction of molecular equilibrium structures by the standard electronic wave functions. Journal of Chemical Physics, 1997, 106, 6430-6440.	1.2	333
239	Principles of direct 4-component relativistic SCF: application to caesium auride. Molecular Physics, 1997, 91, 937-950.	0.8	169
240	Basis-set convergence of correlated calculations on water. Journal of Chemical Physics, 1997, 106, 9639-9646.	1.2	2,197
241	Extensive relativistic calculations on the palladium hydride molecule. Journal of Chemical Physics, 1997, 107, 5496-5501.	1.2	13
242	The Cotton-Mouton effect of liquid water. Part I: The dielectric continuum model. Journal of Chemical Physics, 1997, 107, 894-901.	1.2	20
243	Mechanisms, energetics and dynamics of a key reaction sequence during the decomposition of nitromethane: HNO + HNO â†' N2O + H2O. Computational and Theoretical Chemistry, 1997, 393, 59-71.	1.5	17
244	Ab initio calculation of the NMR shielding and indirect spin-spin coupling constants of fluoroethylene. Molecular Physics, 1997, 91, 881-890.	0.8	27
245	A systematic ab initio study of the water dimer in hierarchies of basis sets and correlation models. Theoretical Chemistry Accounts, 1997, 97, 150-157.	0.5	184
246	Multiple basis sets in calculations of triples corrections in coupled-cluster theory. Theoretical Chemistry Accounts, 1997, 97, 164-176.	0.5	82
247	Cotton-Mouton effect and shielding polarizabilities of ethylene: An MCSCF study. Chemical Physics, 1997, 216, 53-66.	0.9	29
248	The magnetizability, rotational g tensor, and quadrupole moment of PF3 revisited. Chemical Physics Letters, 1997, 264, 17-23.	1.2	46
249	The magnetizability anisotropy and rotational g factor of deuterium hydride and the deuterium molecule. Chemical Physics Letters, 1997, 271, 163-166.	1.2	14
250	CCSDT calculations of molecular equilibrium geometries. Chemical Physics Letters, 1997, 274, 235-241.	1.2	73
251	Electric and magnetic properties of the nitroethene molecule. Molecular Physics, 1997, 92, 89-96.	0.8	3
252	Ab initio calculation of the NMR shielding and indirect spin-spin coupling constants of fluoroethylene. Molecular Physics, 1997, 91, 881-889.	0.8	16

#	Article	IF	Citations
253	Perturbationâ€dependent atomic orbitals for the calculation of spinâ€rotation constants and rotational g tensors. Journal of Chemical Physics, 1996, 105, 2804-2812.	1.2	201
254	Largeâ€scale calculations of excitation energies in coupled cluster theory: The singlet excited states of benzene. Journal of Chemical Physics, 1996, 105, 6921-6939.	1.2	182
255	Full CI calculations of the magnetizability and rotational g factor of the hydrogen molecule. Computational and Theoretical Chemistry, 1996, 388, 231-235.	1.5	17
256	Ab Initio Studies of the [AX]2 Spin Systems ofcis- andtrans-N2F2. , 1996, 34, 646-649.		11
257	Long-range effects of interatomic interactions on NMR shielding constants. Chemical Physics Letters, 1996, 250, 1-8.	1.2	19
258	Efficient parallel implementation of response theory: Calculations of the second hyperpolarizability of polyacenes. Chemical Physics Letters, 1996, 253, 1-7.	1.2	47
259	Magnetizability and nuclear shielding constants of solvated water. Chemical Physics Letters, 1996, 253, 443-447.	1.2	58
260	Integral direct calculation of CC2 excitation energies: singlet excited states of benzene. Chemical Physics Letters, 1996, 263, 530-539.	1.2	53
261	The molecular structure of ferrocene. Journal of Chemical Physics, 1996, 104, 9528-9530.	1.2	98
262	The integralâ€direct coupled cluster singles and doubles model. Journal of Chemical Physics, 1996, 104, 4157-4165.	1.2	154
263	MCSCF calculations of hypermagnetizabilities and nuclear shielding polarizabilities of CO and CH₄. Molecular Physics, 1996, 88, 931-947.	0.8	39
264	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
265	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
266	Full CI calculations of the magnetizability and rotational g factor of the hydrogen molecule. Computational and Theoretical Chemistry, 1996, 388, 231-235.	1.5	10
267	Loss of H2 from CH3NH3+, CH3OH2+ and CH3FH+. Reaction mechanisms and dynamics from observation of metastable ion fragmentations and ab initio calculations. European Journal of Mass Spectrometry, 1995, 1, 121.	0.7	12
268	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
269	A numerically stable orbital connection for the calculation of analytical Hessians using perturbation-dependent basis sets. Chemical Physics Letters, 1995, 235, 47-52.	1.2	27
270	NMR properties of N3â˜. A comparison of theory and experiment. Chemical Physics Letters, 1995, 243, 144-150.	1.2	9

#	Article	IF	Citations
271	Accurate magnetizabilities of the isoelectronic series BeHâ^', BH, and CH+. The MCSCF-GIAO approach. Chemical Physics, 1995, 195, 157-169.	0.9	77
272	Orbital connections for perturbation-dependent basis sets. Theoretica Chimica Acta, 1995, 90, 421-439.	0.9	67
273	Random-phase calculations of frequency-dependent polarizabilities and hyperpolarizabilities of long polyene chains. Physical Review B, 1995, 51, 14949-14957.	1.1	31
274	SCF calculations of the NMR shielding tensor for the ethylenic carbon atom in C3Cl4. Molecular Physics, 1995, 85, 671-673.	0.8	6
275	Ab initio calculation of electronic circular dichroism fortrans-cyclooctene using London atomic orbitals. Theoretica Chimica Acta, 1995, 90, 441-458.	0.9	46
276	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.	1.2	89
277	GAUSSIAN BASIS SETS AND MOLECULAR INTEGRALS. Advanced Series in Physical Chemistry, 1995, , 725-856.	1.5	59
278	Second-Order Methods for the Optimization of Molecular Potential Energy Surfaces. , 1995, , 109-136.		2
279	Orbital connections for perturbation-dependent basis sets. Theoretica Chimica Acta, 1995, 90, 421.	0.9	33
280	Ab initio. Theoretica Chimica Acta, 1995, 90, 441.	0.9	86
281	Multiconfigurational selfâ€consistent field calculations of nuclear shieldings using London atomic orbitals. Journal of Chemical Physics, 1994, 100, 8178-8185.	1.2	229
282	MCSCF reaction-path energetics and thermal rate-constants for the reaction of3NH with H2. Theoretica Chimica Acta, 1994, 89, 157-168.	0.9	6
283	MCSCF calculations of nitrogen NMR shielding constants using London atomic orbitals. Chemical Physics Letters, 1994, 220, 154-160.	1.2	18
284	MCSCF calculations of Verdet constants. Chemical Physics Letters, 1994, 222, 263-266.	1.2	29
285	Theoretical calculations of the magnetizability of some small fluorine-containing molecules using London atomic orbitals. Chemical Physics Letters, 1994, 223, 12-18.	1.2	30
286	An ab initio nuclear magnetic resonance spectrum of vinyllithium. Chemical Physics Letters, 1994, 226, 1-10.	1.2	16
287	A direct atomic orbital driven implementation of the coupled cluster singles and doubles (CCSD) model. Chemical Physics Letters, 1994, 228, 233-238.	1.2	126
288	The Vegard-Kaplan band and the phosphorescent decay of N2. Chemical Physics Letters, 1994, 231, 387-394.	1.2	8

#	Article	IF	Citations
289	Frequencyâ€dependent polarizabilities of O2 and van der Waals coefficients of dimers containing O2. Journal of Chemical Physics, 1994, 100, 1297-1302.	1.2	48
290	Vibrational Raman optical activity calculations using London atomic orbitals. Faraday Discussions, 1994, 99, 165-180.	1.6	225
291	Magnetizability of Hydrocarbons. Journal of the American Chemical Society, 1994, 116, 10135-10140.	6.6	73
292	Multiconfigurational selfâ€consistent field calculations of nuclear magnetic resonance indirect spinâ€“spin coupling constants. Journal of Chemical Physics, 1994, 101, 6822-6828.	1.2	29
293	Basis set convergence of atomic axial tensors obtained from selfâ€consistent field calculations using London atomic orbitals. Journal of Chemical Physics, 1994, 100, 6620-6627.	1.2	28
294	Basis set convergence and correlation effects in vibrational circular dichroism calculations using London atomic orbitals. Faraday Discussions, 1994, 99, 121-129.	1.6	32
295	Mechanism, energetics, kinetics and dynamics of the reaction C2H6+Ë™ â† ' C2H4+Ë™ + H2. Organic Mass Spectrometry, 1993, 28, 1262-1269.	1.3	19
296	The nuclear spinâ€"spin coupling in N2 and CO. Chemical Physics Letters, 1993, 209, 201-206.	1.2	38
297	Nuclear magnetic shielding tensor for the ethylenic carbon atom in tetrachlorocyclopropene. Chemical Physics Letters, 1993, 204, 608-610.	1.2	9
298	Ab initio study of the NMR shielding constants and spin-spin coupling constants in cyclopropene. Theoretica Chimica Acta, 1993, 87, 19-28.	0.9	21
299	Large scale random phase calculations for direct self-consistent field wavefunctions. Chemical Physics, 1993, 172, 13-20.	0.9	29
300	Gaugeâ€origin independent multiconfigurational selfâ€consistentâ€field theory for vibrational circular dichroism. Journal of Chemical Physics, 1993, 98, 8873-8887.	1.2	186
301	Frequency dependent hyperpolarizabilities of polyynes. Journal of Chemical Physics, 1993, 98, 7229-7235.	1.2	31
302	Hartreeâ€"Fock limit magnetizabilities from London orbitals. Journal of Chemical Physics, 1993, 99, 3847-3859.	1.2	202
303	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.	1.2	94
304	The hydrogen atom in crossed static electromagnetic and non-resonant laser fields. Physica Scripta, 1992, 46, 354-356.	1.2	4
305	Calculation of Geometrical Derivatives in Molecular Electronic Structure Theory. NATO ASI Series Series B: Physics, 1992, , 353-421.	0.2	49
306	Spin polarization in restricted electronic structure theory: Multiconfiguration selfâ€consistentâ€field calculations of hyperfine coupling constants. Journal of Chemical Physics, 1992, 97, 3412-3419.	1.2	46

#	Article	IF	Citations
307	Spinâ€“orbit coupling constants in a multiconfiguration linear response approach. Journal of Chemical Physics, 1992, 96, 2118-2126.	1.2	90
308	Firstâ€order nonadiabatic coupling matrix elements from multiconfigurational selfâ€consistentâ€field response theory. Journal of Chemical Physics, 1992, 97, 7573-7584.	1.2	31
309	Multiconfigurational quadratic response functions for singlet and triplet perturbations: The phosphorescence lifetime of formaldehyde. Journal of Chemical Physics, 1992, 97, 9178-9187.	1.2	148
310	Interconversion of diborane (4) isomers. Journal of Chemical Physics, 1992, 97, 1211-1216.	1.2	33
311	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.	6.6	141
312	Indirect nuclear spinâ€“spin coupling constants from multiconfiguration linear response theory. Journal of Chemical Physics, 1992, 96, 6120-6125.	1.2	147
313	The second-order energy contribution from the spin-orbit interaction operator to the potential energy curve of Cr2. International Journal of Quantum Chemistry, 1992, 41, 729-731.	1.0	5
314	On the evaluation of derivatives of Gaussian integrals. Theoretica Chimica Acta, 1992, 83, 177-183.	0.9	36
315	The magnetic hyperpolarizability anisotropy of the neon atom. Chemical Physics Letters, 1992, 191, 599-602.	1.2	17
316	Optimization of Minima and Saddle Points. Lecture Notes in Quantum Chemistry II, 1992, , 295-324.	0.3	2
317	Excited state structures and vibronic spectra of H2CO+, HDCO+, and D2CO+ using molecular gradient and Hessian techniques. Journal of Chemical Physics, 1991, 95, 5906-5917.	1.2	14
318	An electronic Hamiltonian for origin independent calculations of magnetic properties. Journal of Chemical Physics, 1991, 95, 2595-2601.	1.2	320
319	An ab initio investigation of the potential energy function and rotationâ€“vibration energies of H2OÂ·Na+. Chemical Physics Letters, 1991, 185, 265-269.	1.2	7
320	Transition-state optimizations by trust-region image minimization. Chemical Physics Letters, 1991, 182, 503-510.	1.2	156
321	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.	1.2	529
322	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.	1.2	254
323	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.	1.2	222
324	Accurate calculations of the dynamic dipole polarizability of N2. A multiconfigurational linear response study using restricted active space (RAS) wavefunctions. Chemical Physics Letters, 1989, 162, 355-360.	1.2	22

#	Article	IF	Citations
325	Configuration-interaction energy derivatives in a fully variational formulation. Theoretica Chimica Acta, 1989, 75, 111-127.	0.9	186
326	A numerically stable procedure for calculating Mï¿½ller-Plesset energy derivatives, derived using the theory of Lagrangians. Theoretica Chimica Acta, 1989, 76, 227-245.	0.9	92
327	A gradient extremal walking algorithm. Theoretica Chimica Acta, 1988, 73, 55-65.	0.9	69
328	Molecular wave functions and properties calculated using floating Gaussian orbitals. Journal of Chemical Physics, 1988, 89, 4889-4902.	1.2	43
329	Mo/llerâ€“Plesset energy derivatives. Journal of Chemical Physics, 1988, 89, 1560-1570.	1.2	190
330	A multiconfigurational selfâ€consistent reactionâ€field method. Journal of Chemical Physics, 1988, 89, 3086-3095.	1.2	198
331	Gaussian basis sets for high-quality ab initio calculations. The Journal of Physical Chemistry, 1988, 92, 3029-3033.	2.9	69
332	Analytical Calculation of Geometrical Derivatives in Molecular Electronic Structure Theory. Advances in Quantum Chemistry, 1988, 19, 183-245.	0.4	167
333	Effect of the Crystalline Environment on Molecular Geometries -- an ab initio Study of Cyanamide.. Acta Chemica Scandinavica, 1988, 42a, 269-272.	0.7	12
334	Translation and Rotational Symmetries of Molecular Geometrical Derivatives.. Acta Chemica Scandinavica, 1988, 42a, 515-518.	0.7	4
335	Ground-state potential energy surface of diazene. Journal of the American Chemical Society, 1987, 109, 2895-2901.	6.6	66
336	Analytical calculation of MCSCF dipoleâ€moment derivatives. Journal of Chemical Physics, 1986, 84, 6280-6284.	1.2	43
337	Systematic determination of MCSCF equilibrium and transition structures and reaction paths. Journal of Chemical Physics, 1986, 85, 3917-3929.	1.2	29
338	Molecular Hessians for largeâ€scale MCSCF wave functions. Journal of Chemical Physics, 1986, 84, 6266-6279.	1.2	109
339	Hamiltonian Expansion in Geometrical Distortions. , 1986, , 1-16.		15
340	Walking on MCSCF Potential Energy Surfaces: Application to H2O2 and NH3. , 1986, , 229-241.		2
341	Calculation of Dipole Moments, Polarizabilities and Their Geometrical Derivatives. , 1986, , 115-133.		1
342	Higher molecular-deformation derivatives of the configuration-interaction energy. Chemical Physics, 1984, 86, 413-432.	0.9	40

#	Article	IF	Citations
343	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.	1.0	82
344	Simple derivation of the potential energy gradient for an arbitrary electronic wave function. International Journal of Quantum Chemistry, 1982, 21, 939-940.	1.0	9
345	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
346	Basis set considerations for the calculation of gradients in the lcao formalism. Chemical Physics Letters, 1981, 83, 125-128.	1.2	8
347	MCSCF calculations of hypermagnetizabilities and nuclear shielding polarizabilities of CO and CH4. , 0, .		6
348	LutosÅ‚aw Wolniewicz (1930â€“2020). Molecular Physics, 0, , .	0.8	0