List of Publications by Year in descending order

184 papers	16,201 citations	23544 58 h-index	16636 123 g-index
187 all docs	187 docs citations	187 times ranked	7125 citing authors

#	Article	IF	Citations
1	Basis-set convergence in correlated calculations on Ne, N2, and H2O. Chemical Physics Letters, 1998, 286, 243-252.	1.2	1,989
2	The second-order approximate coupled cluster singles and doubles model CC2. Chemical Physics Letters, 1995, 243, 409-418.	1.2	1,564
3	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	6.2	1,166
4	Basis-set convergence of the energy in molecular Hartreeâ€“Fock calculations. Chemical Physics Letters, 1999, 302, 437-446.	1.2	604
5	Recent Advances in Wave Function-Based Methods of Molecular-Property Calculations. Chemical Reviews, 2012, 112, 543-631.	23.0	549
6	Response functions from Fourier component variational perturbation theory applied to a time-averaged quasienergy. International Journal of Quantum Chemistry, 1998, 68, 1-52.	1.0	497
7	Polarization propagator methods in atomic and molecular calculations. Computer Physics Reports, 1984, 2, 33-92.	2.3	387
8	The accurate determination of molecular equilibrium structures. Journal of Chemical Physics, 2001, 114, 6548-6556.	1.2	353
9	Passing the one-billion limit in full configuration-interaction (FCI) calculations. Chemical Physics Letters, 1990, 169, 463-472.	1.2	326
10	Molecular equilibrium structures from experimental rotational constants and calculated vibrationâ€“rotation interaction constants. Journal of Chemical Physics, 2002, 116, 6482-6496.	1.2	245
11	Excitation energies of BH, CH2 and Ne in full configuration interaction and the hierarchy CCS, CC2, CCSD and CC3 of coupled cluster models. Chemical Physics Letters, 1995, 244, 75-82.	1.2	232
12	Vibrational Raman optical activity calculations using London atomic orbitals. Faraday Discussions, 1994, 99, 165-180.	1.6	225
13	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
14	Excitation energies of H2O, N2 and C2 in full configuration interaction and coupled cluster theory. Chemical Physics Letters, 1996, 256, 185-194.	1.2	218
15	Highly accurate calculations of molecular electronic structure. Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, R103-R130.	0.6	214
16	A priori calculation of molecular properties to chemical accuracy. Journal of Physical Organic Chemistry, 2004, 17, 913-933.	0.9	204
17	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
18	A multiconfigurational time-dependent hartree-fock approach. Chemical Physics Letters, 1979, 65, 77-80.	1.2	175

#	Article	IF	Citations
19	The Equilibrium Structure of Ferrocene. ChemPhysChem, 2006, 7, 245-249.	1.0	149
20	Linear scaling coupled cluster method with correlation energy based error control. Journal of Chemical Physics, 2010, 133, 014107.	1.2	147
21	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
22	Weak Intramolecular Interactions in Ethylene Glycol Identified by Vapor Phase OHâ"Stretching Overtone Spectroscopy. Journal of the American Chemical Society, 2005, 127, 17096-17103.	6.6	135
23	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
24	Frequency-dependent first hyperpolarizabilities using coupled cluster quadratic response theory. Chemical Physics Letters, 1997, 269, 428-434.	1.2	125
25	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
26	The accuracy ofab initiomolecular geometries for systems containing second-row atoms. Journal of Chemical Physics, 2005, 123, 184107.	1.2	125
27	Full configuration interaction benchmarking of coupled-cluster models for the lowest singlet energy surfaces of N2. Journal of Chemical Physics, 2000, 113, 6677-6686.	1.2	109
28	Frequency-dependent second hyperpolarizabilities using coupled cluster cubic response theory. Chemical Physics Letters, 1998, 282, 139-146.	1.2	108
29	Optimization and Characterization of a Multiconfigurational Self-Consistent Field (MCSCF) State. Advances in Chemical Physics, 2007, , 1-176.	0.3	108
30	Excitation energies, transition moments and dynamic polarizabilities for CH+. A comparison of multiconfigurational linear response and full configuration interaction calculations. Chemical Physics Letters, 1989, 154, 380-386.	1.2	107
31	A density matrix-based quasienergy formulation of the Kohnâ€"Sham density functional response theory using perturbation- and time-dependent basis sets. Journal of Chemical Physics, 2008, 129, 214108.	1.2	99
32	Coupled cluster calculations of the optical rotation of S-propylene oxide in gas phase and solution. Chemical Physics Letters, 2005, 401, 385-392.	1.2	94
33	A Locality Analysis of the Divideâ€"Expandâ€"Consolidate Coupled Cluster Amplitude Equations. Journal of Chemical Theory and Computation, 2011, 7, 1677-1694.	2.3	93
34	Linear-scaling implementation of molecular response theory in self-consistent field electronic-structure theory. Journal of Chemical Physics, 2007, 126, 154108.	1.2	87
35	Ab initio. Theoretica Chimica Acta, 1995, 90, 441.	0.9	86
36	Local orbitals by minimizing powers of the orbital variance. Journal of Chemical Physics, 2011, 134, 194104.	1.2	82

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37	The divide-expand-consolidate family of coupled cluster methods: Numerical illustrations using second order MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2012, 136, 014105.	1.2	80
38	On the inherent divergence in the MÃ¸ller-Plesset series. The neon atom â€" a test case. Chemical Physics Letters, 1996, 261, 369-378.	1.2	79
39	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
40	Linear-scaling implementation of molecular electronic self-consistent field theory. Journal of Chemical Physics, 2007, 126, 114110.	1.2	78
41	Accurate magnetizabilities of the isoelectronic series BeHâ^', BH, and CH+. The MCSCF-GIAO approach. Chemical Physics, 1995, 195, 157-169.	0.9	77
42	Accuracy of spectroscopic constants of diatomic molecules from ab initio calculations. Journal of Chemical Physics, 2003, 118, 2539.	1.2	77
43	Linear-Scaling Coupled Cluster with Perturbative Triple Excitations: The Divideâ€"Expandâ€"Consolidate CCSD(T) Model. Journal of Chemical Theory and Computation, 2015, 11, 2984-2993.	2.3	77
44	Triplet excitation energies in full configuration interaction and coupled-cluster theory. Journal of Chemical Physics, 2001, 115, 3015-3020.	1.2	76
45	The Electronic Spectrum of Furan. Journal of the American Chemical Society, 1998, 120, 3423-3430.	6.6	74
46	CCSDT calculations of molecular equilibrium geometries. Chemical Physics Letters, 1997, 274, 235-241.	1.2	73
47	Direct optimization of the AO density matrix in Hartreeâ€"Fock and Kohnâ€"Sham theories. Chemical Physics Letters, 2000, 327, 397-403.	1.2	72
48	Response Theory and Calculations of Molecular Hyperpolarizabilities. Advances in Quantum Chemistry, 1995, 26, 165-237.	0.4	71
49	Orbital localization using fourth central moment minimization. Journal of Chemical Physics, 2012, 137, 224114.	1.2	71
50	A gradient extremal walking algorithm. Theoretica Chimica Acta, 1988, 73, 55-65.	0.9	69
51	Coupled-cluster connected-quadruples corrections to atomization energies. Chemical Physics Letters, 2003, 371, 62-67.	1.2	68
52	Comparison of coupled-cluster and Brueckner coupled-cluster calculations of molecular properties. Chemical Physics Letters, 1993, 211, 94-100.	1.2	67
53	The accuracy of molecular dipole moments in standard electronic structure calculations. Chemical Physics Letters, 2000, 319, 563-568.	1.2	67
54	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

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55	Ab initio determinations of magnetic circular dichroism. Chemical Physics Letters, 1999, 300, 61-68.	1.2	66
56	Gauge-origin independent magneto-optical activity within coupled cluster response theory. Journal of Chemical Physics, 2000, 113, 3561-3572.	1.2	64
57	On the Efficiency of Algorithms for Solving Hartreeâ€“Fock and Kohnâ€“Sham Response Equations. Journal of Chemical Theory and Computation, 2011, 7, 1610-1630.	2.3	64
58	Trust Region Minimization of Orbital Localization Functions. Journal of Chemical Theory and Computation, 2012, 8, 3137-3146.	2.3	64
59	Quasienergy formulation of damped response theory. Journal of Chemical Physics, 2009, 131, 044112.	1.2	63
60	Proper characterization of MC SCF stationary points. Chemical Physics, 1983, 78, 175-199.	0.9	59
61	Coupled-cluster singles, doubles and triples (CCSDT) calculations of atomization energies. Chemical Physics Letters, 2000, 317, 116-122.	1.2	58
62	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
63	MP2 energy and density for large molecular systems with internal error control using the Divide-Expand-Consolidate scheme. Physical Chemistry Chemical Physics, 2012, 14, 15706.	1.3	57
64	The molecular electric quadrupole moment of N2. Chemical Physics Letters, 1998, 294, 292-296.	1.2	56
65	Calculation of frequency-dependent polarizabilities using the approximate coupled-cluster triples model CC3. Journal of Chemical Physics, 2003, 118, 1292-1300.	1.2	56
66	Integral direct calculation of CC2 excitation energies: singlet excited states of benzene. Chemical Physics Letters, 1996, 263, 530-539.	1.2	53
67	Ab initiostudy of magnetochiral birefringence. Journal of Chemical Physics, 2002, 117, 6417-6428.	1.2	51
68	A numerical study of the convergency of second and approximate second-order multiconfiguration Hartree-Fock procedures. Molecular Physics, 1980, 39, 587-596.	0.8	50
69	Characterization and Generation of Local Occupied and Virtual Hartreeâ€“Fock Orbitals. Chemical Reviews, 2016, 116, 3306-3327.	23.0	48
70	High-order correlation effects on dynamic hyperpolarizabilities and their geometric derivatives: A comparison with density functional results. Journal of Chemical Physics, 2006, 124, 114101.	1.2	46
71	An analysis and implementation of a general coupled cluster approach to excitation energies with application to the B2 molecule. Journal of Chemical Physics, 2001, 115, 671-679.	1.2	45
72	The augmented Roothaanâ€“Hall method for optimizing Hartreeâ€“Fock and Kohnâ€“Sham density matrices. Journal of Chemical Physics, 2008, 129, 124106.	1.2	45

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73	Coupled-cluster theory in a projected atomic orbital basis. Journal of Chemical Physics, 2006, 124, 084103.	1.2	44
74	Molecular gradient for second-order MÃ¸ller-Plesset perturbation theory using the divide-expand-consolidate (DEC) scheme. Journal of Chemical Physics, 2012, 137, 114102.	1.2	43
75	Pipekâ€“Mezey localization of occupied and virtual orbitals. Journal of Computational Chemistry, 2013, 34, 1456-1462.	1.5	43
76	Frequency-dependent hyperpolarizability of hydrogen fluoride. Chemical Physics Letters, 1992, 191, 293-298.	1.2	42
77	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
78	Damped response theory description of two-photon absorption. Journal of Chemical Physics, 2011, 134, 214104.	1.2	42
79	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
80	Higher molecular-deformation derivatives of the configuration-interaction energy. Chemical Physics, 1984, 86, 413-432.	0.9	40
81	Triplet excitation energies in the coupled cluster singles and doubles model using an explicit triplet spin coupled excitation space. Journal of Chemical Physics, 2000, 113, 7765-7772.	1.2	40
82	Linear-scaling symmetric square-root decomposition of the overlap matrix. Journal of Chemical Physics, 2007, 126, 124104.	1.2	40
83	Maximum locality in occupied and virtual orbital spaces using a least-change strategy. Journal of Chemical Physics, 2009, 131, 124112.	1.2	40
84	A Lagrangian framework for deriving triples and quadruples corrections to the CCSD energy. Journal of Chemical Physics, 2014, 140, 064108.	1.2	40
85	Determination of excitation energies and transition moments in a second order polarization propagator approach. Application to the Be atom and the CH+molecule. International Journal of Quantum Chemistry, 1977, 12, 655-670.	1.0	39
86	The divideâ€“expandâ€“consolidate MP2 scheme goes massively parallel. Molecular Physics, 2013, 111, 1196-1210.	0.8	38
87	Ground and excited state polarizabilities and dipole transition properties of benzene from coupled cluster response theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1999, 55, 509-524.	2.0	37
88	Gauge-Origin Independent Formulation and Implementation of Magneto-Optical Activity within Atomic-Orbital-Density Based Hartreeâ^'Fock and Kohnâ^'Sham Response Theories. Journal of Chemical Theory and Computation, 2009, 5, 1997-2020.	2.3	37
89	Coupled hartree-fock and second order polarization propagator calculations of indirect nuclear spin-spin coupling constants for diatomic molecules. Chemical Physics, 1977, 25, 451-458.	0.9	36
90	Geometrical derivatives and magnetic properties in atomic-orbital density-based Hartreeâ€“Fock theory. Journal of Chemical Physics, 2001, 115, 10344.	1.2	36

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91	Multiple stationary point representations in MC SCF calculations. Chemical Physics, 1985, 93, 83-100.	0.9	35
92	Efficient elimination of response parameters in molecular property calculations for variational and nonvariational energies. Journal of Chemical Physics, 2008, 129, 214103.	1.2	35
93	Singlet excited states of Be2. Journal of Chemical Physics, 2000, 112, 3671-3679.	1.2	34
94	The hyperpolarizability of the Ne atom in the approximate coupled cluster triples model CC3. Chemical Physics Letters, 2004, 391, 27-32.	1.2	34
95	Indirect nuclear spin-spin coupling constants within the coupled multiconfiguration hartree-fock approximation. Chemical Physics Letters, 1980, 76, 354-358.	1.2	33
96	Orbital connections for perturbation-dependent basis sets. Theoretica Chimica Acta, 1995, 90, 421.	0.9	33
97	Basis set convergence and correlation effects in vibrational circular dichroism calculations using London atomic orbitals. Faraday Discussions, 1994, 99, 121-129.	1.6	32
98	Implementation of electronic ground states and singlet and triplet excitation energies in coupled cluster theory with approximate triples corrections. Journal of Chemical Physics, 2002, 116, 5963-5970.	1.2	32
99	Linear response CC2 triplet excitation energies. Chemical Physics Letters, 2000, 328, 291-301.	1.2	31
100	The trust-region self-consistent field method in Kohnâ€“Sham density-functional theory. Journal of Chemical Physics, 2005, 123, 074103.	1.2	31
101	Response theory calculations of the vibronically induced 1A1gâ^'1B2u two-photon spectrum of benzene. Chemical Physics Letters, 1993, 209, 513-518.	1.2	30
102	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
103	On the divergent behavior of MÃ¸llerâ€“Plesset perturbation theory for the molecular electric dipole moment. Journal of Chemical Physics, 2000, 112, 1107-1112.	1.2	30
104	General biorthogonal projected bases as applied to second-order MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2007, 127, 074106.	1.2	30
105	Large scale random phase calculations for direct self-consistent field wavefunctions. Chemical Physics, 1993, 172, 13-20.	0.9	29
106	MCSCF calculations of Verdet constants. Chemical Physics Letters, 1994, 222, 263-266.	1.2	29
107	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
108	Quadratic Response Functions in a Second-Order Polarization Propagator Frameworkâ€. Journal of Physical Chemistry A, 2005, 109, 11618-11628.	1.1	29

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109	Molecular response properties from a Hermitian eigenvalue equation for a time-periodic Hamiltonian. Journal of Chemical Physics, 2015, 142, 114109.	1.2	29
110	Molecular response properties in equation of motion coupled cluster theory: A time-dependent perspective. Journal of Chemical Physics, 2016, 144, 024102.	1.2	29
111	Frequency-dependent polarizabilities and second hyperpolarizabilities of N2. Chemical Physics Letters, 1993, 205, 555-562.	1.2	28
112	An Atomic-Orbital-Based Lagrangian Approach for Calculating Geometric Gradients of Linear Response Properties. Journal of Chemical Theory and Computation, 2010, 6, 1028-1047.	2.3	28
113	Geometrical derivatives of dipole moments and polarizabilities. International Journal of Quantum Chemistry, 1984, 25, 1135-1150.	1.0	27
114	A perspective on the localizability of Hartreeâ€“Fock orbitals. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	25
115	Selection of configurations for SCF-CI calculations of spectral properties and comparison with TDHF calculations. Theoretica Chimica Acta, 1974, 32, 203-216.	0.9	24
116	Two-particle, two-hole corrections to a self-consistent time-dependent Hartreeâ€”Fock scheme. Chemical Physics Letters, 1975, 32, 111-115.	1.2	24
117	A basis set study of coupled cluster and full configuration interaction calculations of molecular electric properties for BH. Chemical Physics Letters, 1998, 291, 536-546.	1.2	24
118	CC3 triplet excitation energies using an explicit spin coupled excitation space. Journal of Chemical Physics, 2001, 115, 3545-3552.	1.2	24
119	Dispersion coefficients for first hyperpolarizabilities using coupled cluster quadratic response theory. Theoretical Chemistry Accounts, 1998, 100, 230-240.	0.5	23
120	On the convergence of perturbative coupled cluster triples expansions: Error cancellations in the CCSD(T) model and the importance of amplitude relaxation. Journal of Chemical Physics, 2015, 142, 014102.	1.2	23
121	Comparison of Two Statistical Approaches to Calculate Atomic and Molecular Orbitals. Physical Review A, 1973, 8, 112-119.	1.0	22
122	Multiconfigurational Hartree-Fock response functions. International Journal of Quantum Chemistry, 1983, 23, 959-971.	1.0	22
123	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
124	Coupled cluster calculations of Verdet constants. Chemical Physics Letters, 1997, 281, 445-451.	1.2	22
125	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
126	Brueckner coupled cluster response functions. International Journal of Quantum Chemistry, 1994, 49, 835-848.	1.0	21

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127	MCSCF calculation of response properties of Argon. Theoretica Chimica Acta, 1995, 90, 291-306.	0.9	21
128	An efficient algorithm for solving nonlinear equations with a minimal number of trial vectors: Applications to atomic-orbital based coupled-cluster theory. Journal of Chemical Physics, 2008, 128, 204105.	1.2	21
129	Triple excitation effects in coupled cluster calculations of Verdet constants. Chemical Physics Letters, 2000, 330, 463-470.	1.2	20
130	Orbital spaces in the divide-expand-consolidate coupled cluster method. Journal of Chemical Physics, 2016, 144, 164116.	1.2	20
131	Benzeneâ€“argon triplet intermolecular potential energy surface. Journal of Chemical Physics, 2003, 119, 4762-4767.	1.2	19
132	Analytic ab initio calculations of coherent anti-Stokes Raman scattering (CARS). Physical Chemistry Chemical Physics, 2009, 11, 2293.	1.3	19
133	The hyperpolarizability of neon revisited. Chemical Physics Letters, 1993, 207, 367-371.	1.2	18
134	MCSCF calculations of nitrogen NMR shielding constants using London atomic orbitals. Chemical Physics Letters, 1994, 220, 154-160.	1.2	18
135	A view on coupled cluster perturbation theory using a bivariational Lagrangian formulation. Journal of Chemical Physics, 2016, 144, 064103.	1.2	18
136	The magnetic hyperpolarizability anisotropy of the neon atom. Chemical Physics Letters, 1992, 191, 599-602.	1.2	17
137	Coupled-cluster calculation of dispersion contributions to interaction energies and polarizabilities. Theoretical Chemistry Accounts, 2001, 106, 251-258.	0.5	17
138	The equilibrium structure of trans-glyoxal from experimental rotational constants and calculated vibrationâ€“rotation interaction constants. Physical Chemistry Chemical Physics, 2003, 5, 5031-5037.	1.3	17
139	Comparison of standard and damped response formulations of magnetic circular dichroism. Journal of Chemical Physics, 2011, 135, 024112.	1.2	17
140	Equation-of-motion coupled cluster perturbation theory revisited. Journal of Chemical Physics, 2014, 140, 174114.	1.2	17
141	An ab initio nuclear magnetic resonance spectrum of vinyllithium. Chemical Physics Letters, 1994, 226, 1-10.	1.2	16
142	An ab initio quartic force field and the fundamental frequencies ofo-benzyne. Chemical Physics Letters, 1994, 228, 568-574.	1.2	16
143	The Cotton-Mouton effect of neon and argon: A benchmark study using highly correlated coupled cluster wave functions. Journal of Chemical Physics, 2004, 121, 9461-9473.	1.2	16
144	A ground-state-directed optimization scheme for the Kohnâ€“Sham energy. Physical Chemistry Chemical Physics, 2008, 10, 5344.	1.3	16

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145	Variational response-function formulation of vibrational circular dichroism. Physical Chemistry Chemical Physics, 2011, 13, 4224.	1.3	16
146	Assessment of the accuracy of coupled cluster perturbation theory for open-shell systems. I. Triples expansions. Journal of Chemical Physics, 2016, 144, 194102.	1.2	16
147	Dispersion coefficients for second hyperpolarizabilities using coupled cluster cubic response theory. Advances in Quantum Chemistry, 1999, , 111-148.	0.4	15
148	Nuclear quadrupole coupling constants in NH4Cl. Physical Chemistry Chemical Physics, 1999, 1, 4165-4168.	1.3	15
149	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
150	Communication: The performance of non-iterative coupled cluster quadruples models. Journal of Chemical Physics, 2015, 143, 041101.	1.2	15
151	Tripletâ€”triplet absorption spectra of alternant hydrocarbons within the grand canonical time-dependent hartreeâ€”fock approximation. Chemical Physics Letters, 1973, 18, 261-267.	1.2	14
152	Comparison of full-configuration interaction and coupled-cluster harmonic and fundamental frequencies for BH and HF. Chemical Physics Letters, 2001, 342, 200-206.	1.2	14
153	Gauge invariance of oscillator strengths in the approximate coupled cluster triples model CC3. Chemical Physics Letters, 2004, 389, 413-420.	1.2	14
154	Discarding Information from Previous Iterations in an Optimal Way To Solve the Coupled Cluster Amplitude Equations. Journal of Chemical Theory and Computation, 2015, 11, 1518-1524.	2.3	14
155	Generalizations of the multiconfigurational time-dependent Hartreeâ€“Fock approach. Faraday Symposia of the Chemical Society, 1984, 19, 85-95.	0.5	13
156	Dynamic CCSD polarisabilities of CHF3 and CHCl3. Chemical Physics Letters, 1996, 253, 373-376.	1.2	13
157	Restricted and complete-active-space multiconfiguration linear response calculations of the polarizability of formamide and urea. Chemical Physics Letters, 1991, 186, 379-385.	1.2	12
158	Radiative lifetimes of triplet spin sublevels of the azabenzenes. Chemical Physics, 1994, 181, 291-304.	0.9	12
159	Frequency-dependent hyperpolarizabilities of the Ne, Ar, and Kr atoms using the approximate coupled cluster triples model CC3. Journal of Chemical Physics, 2005, 123, 094303.	1.2	12
160	Robust and Reliable Multilevel Minimization of the Kohnâ^'Sham Energy. Journal of Chemical Theory and Computation, 2009, 5, 1027-1032.	2.3	12
161	The same number of optimized parameters scheme for determining intermolecular interaction energies. Journal of Chemical Physics, 2015, 142, 114116.	1.2	12
162	The second hyperpolarizability of the N2 molecule calculated using the approximate coupled cluster triples model CC3. Chemical Physics Letters, 2005, 413, 272-279.	1.2	11

#	Article	IF	Citations
163	Quartic coupled cluster force fields for the diazene isomers. Chemical Physics Letters, 1993, 215, 576-581.	1.2	10
164	Local Hartreeâ€“Fock orbitals using a threeâ€level optimization strategy for the energy. Journal of Computational Chemistry, 2013, 34, 1311-1320.	1.5	10
165	Dipole polarizability surfaces of ammonia. Chemical Physics, 1990, 144, 343-351.	0.9	9
166	Nuclear magnetic shielding tensor for the ethylenic carbon atom in tetrachlorocyclopropene. Chemical Physics Letters, 1993, 204, 608-610.	1.2	9
167	NMR properties of N3â^'. A comparison of theory and experiment. Chemical Physics Letters, 1995, 243, 144-150.	1.2	9
168	Calculation of first-order one-electron properties using the coupled-cluster approximate triples model CC3. Physical Chemistry Chemical Physics, 2002, 4, 5221-5226.	1.3	9
169	Localized orbitals from basis sets augmented with diffuse functions. Journal of Chemical Physics, 2013, 138, 204104.	1.2	9
170	The Vegard-Kaplan band and the phosphorescent decay of N2. Chemical Physics Letters, 1994, 231, 387-394.	1.2	8
171	Coupled cluster calculations of the polarizability of furan. Chemical Physics Letters, 1997, 281, 438-444.	1.2	8
172	Calculation of ground and excited state potential energy curves of the MgAr complex using the coupled cluster approximate triples model CC3. Chemical Physics Letters, 2002, 364, 402-408.	1.2	8
173	Generalising localisation schemes of orthogonal orbitals to the localisation of non-orthogonal orbitals. Molecular Physics, 2017, 115, 16-25.	0.8	8
174	Lowest order corrections to excitation energies. Chemical Physics Letters, 1977, 47, 61-64.	1.2	7
175	Evaluation of hyperfine coupling tensors of the BeH and BeF radicals. Chemical Physics Letters, 1995, 232, 463-471.	1.2	7
176	Coupled cluster investigation of Sternheimer shieldings and electric field gradient polarizabilities. Journal of Chemical Physics, 2000, 113, 1688-1697.	1.2	7
177	SCF calculations of the NMR shielding tensor for the ethylenic carbon atom in C3Cl4. Molecular Physics, 1995, 85, 671-673.	0.8	6
178	Estimate of the experimental static hyperpolarizability of neon based on coupled cluster response calculations. Chemical Physics Letters, 1998, 283, 109-113.	1.2	6
179	Orbital nonrelaxed coupled cluster singles and doubles with perturbative triples corrections calculations of first-order one-electron properties. Journal of Chemical Physics, 2002, 117, 9983-9990.	1.2	6
180	Assessment of the accuracy of coupled cluster perturbation theory for open-shell systems. II. Quadruples expansions. Journal of Chemical Physics, 2016, 144, 194103.	1.2	6

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181	The electronic spectra of conjugated free radicals. Molecular Physics, 1973, 26, 725-734.	0.8	5
182	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
183	Cauchy Moments of Ne, Ar, and Kr Atoms Calculated Using the Approximate Coupled Cluster Triples Model CC3. Advances in Quantum Chemistry, 2005, , 9-21.	0.4	3
184	Ab initio potential energy function and geometry of the state of ammonia. Journal of Molecular Spectroscopy, 1992, 152, 199-204.	0.4	2