Rodney J Bartlett

List of Publications by Year
in descending order

587 papers	58,339 citations	1237 110 h-index	1505 219 g-index
606 all docs	606 docs citations	606 times ranked	12025 citing authors

#	Article	IF	Citations
1	A full coupledâ€cluster singles and doubles model: The inclusion of disconnected triples. Journal of Chemical Physics, 1982, 76, 1910-1918.	3.0	5,682
2	Coupled-cluster theory in quantum chemistry. Reviews of Modern Physics, 2007, 79, 291-352.	45.6	2,555
3	The equation of motion coupledâ€cluster method. A systematic biorthogonal approach to molecular excitation energies, transition probabilities, and excited state properties. Journal of Chemical Physics, 1993, 98, 7029-7039.	3.0	2,168
4	Coupledâ€cluster methods with noniterative triple excitations for restricted openâ€shell Hartreeâ€“Fock and other general single determinant reference functions. Energies and analytical gradients. Journal of Chemical Physics, 1993, 98, 8718-8733.	3.0	1,854
5	Many-body perturbation theory, coupled-pair many-electron theory, and the importance of quadruple excitations for the correlation problem. International Journal of Quantum Chemistry, 1978, 14, 561-581.	2.0	1,418
6	Coupled-cluster approach to molecular structure and spectra: a step toward predictive quantum chemistry. The Journal of Physical Chemistry, 1989, 93, 1697-1708.	2.9	1,170
7	The full CCSDT model for molecular electronic structure. Journal of Chemical Physics, 1987, 86, 7041-7050.	3.0	1,119
8	Towards a full CCSDT model for electron correlation. Journal of Chemical Physics, 1985, 83, 4041-4046.	3.0	843
9	Non-iterative fifth-order triple and quadruple excitation energy corrections in correlated methods. Chemical Physics Letters, 1990, 165, 513-522.	2.6	798
10	A linear response, coupled-cluster theory for excitation energy. International Journal of Quantum Chemistry, 1984, 26, 255-265.	2.0	618
11	The equation-of-motion coupled-cluster method: Excitation energies of Be and CO. Chemical Physics Letters, 1989, 164, 57-62.	2.6	582
12	Equation of motion coupled cluster method for electron attachment. Journal of Chemical Physics, 1995, 102, 3629-3647.	3.0	514
13	An open-shell spin-restricted coupled cluster method: application to ionization potentials in nitrogen. The Journal of Physical Chemistry, 1988, 92, 3033-3036.	2.9	511
14	Analytic energy derivatives in manyâ€body methods. I. First derivatives. Journal of Chemical Physics, 1989, 90, 1752-1766.	3.0	509
15	A coupled cluster approach with triple excitations. Journal of Chemical Physics, 1984, 81, 5906-5912.	3.0	440
16	Multi-reference averaged quadratic coupled-cluster method: a size-extensive modification of multi-reference CI. Chemical Physics Letters, 1993, 214, 481-488.	2.6	427
17	Multireference Nature of Chemistry: The Coupled-Cluster View. Chemical Reviews, 2012, 112, 182-243.	47.7	422
18	The equation-of-motion coupled-cluster method. Applications to open- and closed-shell reference states. Chemical Physics Letters, 1993, 207, 414-423.	2.6	407

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19	The ACES II program system. International Journal of Quantum Chemistry, 1992, 44, 879-894.	2.0	404
20	The coupledâ€cluster single, double, triple, and quadruple excitation method. Journal of Chemical Physics, 1992, 97, 4282-4288.	3.0	390
21	Molecular Applications of Coupled Cluster and Many-Body Perturbation Methods. Physica Scripta, 1980, 21, 255-265.	2.5	359
22	Frequency dependent nonlinear optical properties of molecules. Journal of Chemical Physics, 1986, 85, 976-989.	3.0	356
23	Manyâ€body perturbation theory applied to electron pair correlation energies. I. Closedâ€shell firstâ€row diatomic hydrides. Journal of Chemical Physics, 1975, 62, 3258-3268.	3.0	354
24	The coupledâ€cluster single, double, and triple excitation model for openâ€shell single reference functions. Journal of Chemical Physics, 1990, 93, 6104-6105.	3.0	330
25	Molecular hyperpolarizabilities. Journal of Chemical Physics, 1993, 98, 3022-3037.	3.0	329
26	The description of N2 and F2 potential energy surfaces using multireference coupled cluster theory. Journal of Chemical Physics, 1987, 86, 887-907.	3.0	315
27	COUPLED-CLUSTER THEORY: AN OVERVIEW OF RECENT DEVELOPMENTS. Advanced Series in Physical Chemistry, 1995, , 1047-1131.	1.5	310
28	Similarity transformed equation-of-motion coupled-cluster theory: Details, examples, and comparisons. Journal of Chemical Physics, 1997, 107, 6812-6830.	3.0	300
29	Coupledâ€cluster theory and its equationâ€ofâ€motion extensions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 126-138.	14.6	289
30	Open-shell analytical energy gradients for triple excitation many-body, coupled-cluster methods: MBPT(4), CCSD+T(CCSD), CCSD(T),and QCISD(T). Chemical Physics Letters, 1992, 200, 1-7.	2.6	285
31	Applications of Post-Hartree-Fock Methods: A Tutorial. Reviews in Computational Chemistry, 2007, , 65-169.	1.5	273
32	Towards a full CCSDT model for electron correlation. CCSDT-n models. Chemical Physics Letters, 1987, 134, 126-132.	2.6	267
33	Electron correlation effects on the theoretical calculation of nuclear magnetic resonance spinâ€“spin coupling constants. Journal of Chemical Physics, 1996, 104, 3290-3305.	3.0	266
34	Exact Exchange Treatment for Molecules in Finite-Basis-Set Kohn-Sham Theory. Physical Review Letters, 1999, 83, 5455-5458.	7.8	266
35	Full configurationâ€“interaction and state of the art correlation calculations on water in a valence doubleâ€zeta basis with polarization functions. Journal of Chemical Physics, 1996, 104, 8007-8015.	3.0	260
36	Recursive intermediate factorization and complete computational linearization of the coupled-cluster single, double, triple, and quadruple excitation equations. Theoretica Chimica Acta, 1991, 80, 387-405.	0.8	257

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37	Coupledâ€cluster calculations of indirect nuclear coupling constants: The importance of nonâ€Fermi contact contributions. Journal of Chemical Physics, 1994, 101, 2186-2191.	3.0	255
38	A new method for excited states: Similarity transformed equation-of-motion coupled-cluster theory. Journal of Chemical Physics, 1997, 106, 6441-6448.	3.0	254
39	Fifth-Order Many-Body Perturbation Theory and Its Relationship to Various Coupled-Cluster Approaches. Advances in Quantum Chemistry, 1986, , 281-344.	0.8	251
40	The quartic force field of H2O determined by manyâ€body methods that include quadruple excitation effects. Journal of Chemical Physics, 1979, 71, 281-291.	3.0	250
41	A theoretical study of the water dimer interaction. Journal of Chemical Physics, 1988, 89, 3662-3673.	3.0	249
42	Coupledâ€cluster openâ€shell analytic gradients: Implementation of the direct product decomposition approach in energy gradient calculations. Journal of Chemical Physics, 1991, 95, 2623-2638.	3.0	248
43	A direct product decomposition approach for symmetry exploitation in manyâ€body methods. I. Energy calculations. Journal of Chemical Physics, 1991, 94, 4334-4345.	3.0	246
44	Economical triple excitation equation-of-motion coupled-cluster methods for excitation energies. Chemical Physics Letters, 1995, 233, 81-87.	2.6	243
45	Many-body perturbation theory with a restricted open-shell Hartreeâ€"Fock reference. Chemical Physics Letters, 1991, 187, 21-28.	2.6	232
46	Coupled-cluster theory for excited electronic states: The full equation-of-motion coupled-cluster single, double, and triple excitation method. Journal of Chemical Physics, 2001, 115, 8263-8266.	3.0	232
47	Molecular applications of multireference coupledâ€cluster methods using an incomplete model space: Direct calculation of excitation energies. Journal of Chemical Physics, 1988, 88, 4357-4366.	3.0	228
48	Coupled-cluster methods with internal and semi-internal triply and quadruply excited clusters: CCSDt and CCSDtq approaches. Journal of Chemical Physics, 1999, 110, 6103-6122.	3.0	228
49	Comparison of high-order many-body perturbation theory and configuration interaction for H2O. Chemical Physics Letters, 1977, 50, 190-198.	2.6	225
50	Approximately extensive modifications of the multireference configuration interaction method: A theoretical and practical analysis. Journal of Chemical Physics, 1995, 103, 3600-3612.	3.0	225
51	Molecular hyperpolarizabilities. I. Theoretical calculations including correlation. Physical Review A, 1979, 20, 1313-1322.	2.5	216
52	A systematic comparison of molecular properties obtained using Hartreeâ€"Fock, a hybrid Hartreeâ€"Fock densityâ€functionalâ€theory, and coupledâ€cluster methods. Journal of Chemical Physics, 1994, 100, 6550-6561.	3.0	214
53	Iterative and non-iterative triple excitation corrections in coupled-cluster methods for excited electronic states: the EOM-CCSDT-3 and EOM-CCSD(Ì‚f) methods. Chemical Physics Letters, 1996, 258, 581-588.	2.6	212
54	A multi-reference coupled-cluster method for molecular applications. Chemical Physics Letters, 1984, 104, 424-430.	2.6	211

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55	Alternative coupled-cluster ansÃtze II. The unitary coupled-cluster method. Chemical Physics Letters, 1989, 155, 133-140.	2.6	211
56	Analytic energy gradients for open-shell coupled-cluster singles and doubles (CCSD) calculations using restricted open-shell Hartreeâ€"Fock (ROHF) reference functions. Chemical Physics Letters, 1991, 182, 207-215.	2.6	209
57	Accurate binding energies of diborane, borane carbonyl, and borazane determined by many-body perturbation theory. Journal of the American Chemical Society, 1979, 101, 2856-2862.	13.7	206
58	Noniterative energy corrections through fifth-order to the coupled cluster singles and doubles method. Journal of Chemical Physics, 1998, 108, 5243-5254.	3.0	205
59	Hyperpolarizabilities of the hydrogen fluoride molecule: A discrepancy between theory and experiment?. Journal of Chemical Physics, 1986, 84, 2726-2733.	3.0	199
60	Multireference coupled-cluster methods using an incomplete model space: Application to ionization potentials and excitation energies of formaldehyde. Chemical Physics Letters, 1987, 137, 273-278.	2.6	188
61	A natural linear scaling coupled-cluster method. Journal of Chemical Physics, 2004, 121, 10935.	3.0	187
62	A multireference coupledâ€cluster study of the ground state and lowest excited states of cyclobutadiene. Journal of Chemical Physics, 1994, 101, 8972-8987.	3.0	186
63	Stability and energetics of metastable molecules: tetraazatetrahedrane (N4), hexaazabenzene (N6), and octaazacubane (N8). The Journal of Physical Chemistry, 1992, 96, 1173-1178.	2.9	185
64	Can optimized effective potentials be determined uniquely?. Journal of Chemical Physics, 2001, 115, 1635-1649.	3.0	184
65	Configuration interaction singles, time-dependent Hartreeâ€"Fock, and time-dependent density functional theory for the electronic excited states of extended systems. Journal of Chemical Physics, 1999, 111, 10774-10786.	3.0	181
66	New perspectives on unitary coupled-cluster theory. International Journal of Quantum Chemistry, 2006, 106, 3393-3401.	2.0	180
67	A study of Be2with manyâ€body perturbation theory and a coupledâ€cluster method including triple excitations. Journal of Chemical Physics, 1984, 80, 4371-4377.	3.0	178
68	Equation-of-motion coupled cluster method with full inclusion of the connected triple excitations for ionized states: IP-EOM-CCSDT. Journal of Chemical Physics, 2003, 118, 1128-1136.	3.0	177
69	The reduced linear equation method in coupled cluster theory.. Journal of Chemical Physics, 1981, 75, 1284-1292.	3.0	176
70	Perturbative corrections to coupled-cluster and equation-of-motion coupled-cluster energies: A determinantal analysis. Journal of Chemical Physics, 2001, 114, 3919-3928.	3.0	168
71	Improving upon CCSD(T): Î›CCSD(T). I. Potential energy surfaces. Journal of Chemical Physics, 2008, 128, 044110.	3.0	166
72	On the choice of orbitals for symmetry breaking problems with application to NO3. Journal of Chemical Physics, 1992, 97, 5554-5559.	3.0	165

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73	An efficient way to include connected quadruple contributions into the coupled cluster method. Journal of Chemical Physics, 1998, 108, 9221-9226.	3.0	164
74	Property evaluation and orbital relaxation in coupled cluster methods. Journal of Chemical Physics, 1987, 87, 502-509.	3.0	163
75	Ab initiodensity functional theory: The best of both worlds?. Journal of Chemical Physics, 2005, 123, 062205.	3.0	160
76	The exchange-correlation potential inab initiodensity functional theory. Journal of Chemical Physics, 2005, 122, 034104.	3.0	159
77	A CCSD (T) investigation of carbonyl oxide and dioxirane. Equilibrium geometries, dipole moments, infrared spectra, heats of formation and isomerization energies. Chemical Physics Letters, 1993, 209, 547-556.	2.6	157
78	Description of coreâ€excitation spectra by the openâ€shell electronâ€attachment equationâ€ofâ€motion coupled cluster method. Journal of Chemical Physics, 1995, 102, 6735-6756.	3.0	156
79	Secondâ€order manyâ€body perturbationâ€theory calculations in extended systems. Journal of Chemical Physics, 1996, 104, 8553-8565.	3.0	155
80	Electron affinities of CO2, OCS, and CS2. Journal of Chemical Physics, 1998, 108, 6756-6762.	3.0	153
81	A theoretical study of linear carbon cluster monoanions, Câ^'n, and dianions, C2â^'n (n=2â€“10). Journal of Chemical Physics, 1992, 97, 3445-3457.	3.0	151
82	A general modelâ€space coupledâ€cluster method using a Hilbertâ€space approach. Journal of Chemical Physics, 1990, 92, 561-567.	3.0	144
83	A multireference coupledâ€cluster method for special classes of incomplete model spaces. Journal of Chemical Physics, 1989, 91, 6187-6194.	3.0	142
84	The inclusion of connected triple excitations in the equationâ€ofâ€motion coupledâ€cluster method. Journal of Chemical Physics, 1994, 101, 3073-3078.	3.0	141
85	Coupledâ€cluster calculations of the excitation energies of ethylene, butadiene, and cyclopentadiene. Journal of Chemical Physics, 1996, 105, 6979-6988.	3.0	141
86	Similarity transformed equation-of-motion coupled-cluster study of ionized, electron attached, and excited states of free base porphin. Journal of Chemical Physics, 1997, 106, 6449-6455.	3.0	141
87	C2V Insertion pathway for BeH2: A test problem for the coupled-cluster single and double excitation model. International Journal of Quantum Chemistry, 1983, 23, 835-845.	2.0	140
88	Abâ€,initio density functional theory: OEP-MBPT(2). A new orbital-dependent correlation functional. Journal of Chemical Physics, 2002, 116, 4415-4425.	3.0	139
89	Equation-of-motion coupled cluster method with full inclusion of connected triple excitations for electron-attached states: EA-EOM-CCSDT. Journal of Chemical Physics, 2003, 119, 1901-1908.	3.0	139
90	Coupledâ€cluster calculations on the C2 molecule and the C+2 and Câ^'2 molecular ions. Journal of Chemical Physics, 1992, 96, 6073-6084.	3.0	138

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91	Hilbert space multireference coupledâ€cluster methods. I. The single and double excitation model. Journal of Chemical Physics, 1991, 95, 8227-8238.	3.0	134
92	Coupled-cluster singles and doubles for extended systems. Journal of Chemical Physics, 2004, 120, 2581-2592.	3.0	132
93	The expectation value coupled-cluster method and analytical energy derivatives. Chemical Physics Letters, 1988, 150, 29-36.	2.6	131
94	Coupled-cluster calculations of the excitation energies of benzene and the azabenzenes. Journal of Chemical Physics, 1997, 106, 6051-6060.	3.0	126
95	Isomers and excitation energies of C4. Journal of Chemical Physics, 1986, 84, 3284-3290.	3.0	125
96	A Hilbert space multi-reference coupled-cluster study of the H4 model system. Theoretica Chimica Acta, 1991, 80, 335-348.	0.8	124
97	Optimized virtual orbital space for highâ€level correlated calculations. Journal of Chemical Physics, 1987, 86, 6314-6324.	3.0	123
98	Adiabatic electron affinities of small superhalogens: LiF2, LiCl2, NaF2, and NaCl2. Journal of Chemical Physics, 1997, 107, 3867-3875.	3.0	122
99	Spin density of radicals by finite field manyâ€body methods. Journal of Chemical Physics, 1985, 82, 4225-4229.	3.0	121
100	The coupled-cluster revolution. Molecular Physics, 2010, 108, 2905-2920.	1.7	121
101	A theoretical study of the valenceâ€and dipoleâ€bound states of the nitromethane anion. Journal of Chemical Physics, 1996, 105, 8785-8792.	3.0	120
102	On the Stability of N5+N5-. Journal of Physical Chemistry A, 2002, 106, 4639-4644.	2.5	120
103	Contributions from electron correlation to the relative stabilities of the tautomers of nucleic acid bases. Journal of the American Chemical Society, 1988, 110, 2353-2358.	13.7	119
104	Coupled-cluster method tailored by configuration interaction. Journal of Chemical Physics, 2005, 123, 074106.	3.0	117
105	High-order coupled-cluster calculations through connected octuple excitations. Chemical Physics Letters, 2000, 321, 216-224.	2.6	114
106	Multireference coupled-cluster theory: The easy way. Journal of Chemical Physics, 2011, 134, 114108.	3.0	114
107	Molecular hyperpolarizabilities. II. A correlated study ofH2O. Physical Review A, 1981, 23, 1594-1599.	2.5	113
108	The 28-Electron Tetraatomic Molecules:â€‰ N4, CN2O, BFN2, C2O2, B2F2, CBFO, C2FN, and BNO2. Challenges for Computational and Experimental Chemistry. The Journal of Physical Chemistry, 1996, 100, 5702-5714.	2.9	113

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109	Relativistic energy levels and bonding in actinide hexaflourides. Journal of Chemical Physics, 1976, 65, 3331-3340.	3.0	112
110	Theory and implementation of the MBPT density matrix. An application to one-electron properties. Chemical Physics Letters, 1988, 147, 359-366.	2.6	112
111	Simplified methods for equation-of-motion coupled-cluster excited state calculations. Chemical Physics Letters, 1996, 248, 189-198.	2.6	112
112	Frozen Natural Orbitals: Systematic Basis Set Truncation for Coupled-Cluster Theory. Collection of Czechoslovak Chemical Communications, 2005, 70, 837-850.	1.0	112
113	The potential energy curve for theX1Î£g+state of Mg2calculated with manyâ€body perturbation theory. Journal of Chemical Physics, 1978, 68, 2114-2124.	3.0	111
114	Predicted NMR Spectra for Ethyl Carbocations: A Fingerprint for Nonclassical Hydrogen-Bridged Structures. Journal of the American Chemical Society, 1995, 117, 8476-8477.	13.7	109
115	Coupled-cluster methods that include connected quadruple excitations, T4: CCSDTQ-1 and Q(CCSDT). Chemical Physics Letters, 1989, 158, 550-555.	2.6	107
116	EOMXCC: A New Coupled-Cluster Method for Electronic Excited States. Advances in Quantum Chemistry, 1999, 34, 295-380.	0.8	107
117	Is fifth-order MBPT enough?. Chemical Physics Letters, 1985, 113, 151-158.	2.6	106
118	A theoretical study of hyperfine coupling constants. Journal of Chemical Physics, 1994, 100, 1425-1434.	3.0	106
119	Multiplicity of many-body wavefunctions using unrestricted Hartree-Fock reference functions. Collection of Czechoslovak Chemical Communications, 1988, 53, 2203-2213.	1.0	104
120	Structure and NMR Spectra of the 2-Norbornyl Carbocation:â€‰ Prediction of 1J(13C13C) for the Bridged, Pentacoordinate Carbon Atom. Journal of the American Chemical Society, 1996, 118, 7849-7850.	13.7	104
121	Transformation of the Hamiltonian in excitation energy calculations: Comparison between Fockâ€space multireference coupledâ€cluster and equationâ€ofâ€motion coupledâ€cluster methods. Journal of Chemical Physics, 1991, 94, 6670-6676.	3.0	103
122	A coupledâ€cluster based effective Hamiltonian method for dynamic electric polarizabilities. Journal of Chemical Physics, 1993, 99, 5178-5183.	3.0	103
123	Alternative ansÃtze in single reference coupledâ€cluster theory. III. A critical analysis of different methods. Journal of Chemical Physics, 1995, 103, 281-298.	3.0	103
124	High-order determinantal equation-of-motion coupled-cluster calculations for electronic excited states. Chemical Physics Letters, 2000, 326, 255-262.	2.6	103
125	Stability and properties of C4isomers. Journal of Chemical Physics, 1988, 89, 3612-3617.	3.0	102
126	Predicted NMR Coupling Constants Across Hydrogen Bonds:â€‰ A Fingerprint for Specifying Hydrogen Bond Type?. Journal of the American Chemical Society, 2000, 122, 3560-3561.	13.7	100

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127	The multireference coupledâ€cluster method in Hilbert space: An incomplete model space application to the LiH molecule. Journal of Chemical Physics, 1991, 95, 4311-4316.	3.0	99
128	Coupled-cluster calculations of the electronic excitation spectrum of free base porphin in a polarized basis. Journal of Chemical Physics, 1998, 108, 6790-6798.	3.0	98
129	Analytic evaluation of energy gradients at the coupledâ€cluster singles and doubles level using quasiâ€restricted Hartreeâ€“Fock openâ€shell reference functions. Journal of Chemical Physics, 1991, 95, 2639-2645.	3.0	96
130	A dressing for the matrix elements of the singles and doubles equationâ€ofâ€motion coupledâ€cluster method that recovers additive separability of excitation energies. Journal of Chemical Physics, 1995, 102, 7490-7498.	3.0	96
131	Hydrogen Bond Types, Binding Energies, and 1H NMR Chemical Shifts. Journal of Physical Chemistry A, 1999, 103, 8121-8124.	2.5	96
132	Frozen natural orbital coupled-cluster theory: Forces and application to decomposition of nitroethane. Journal of Chemical Physics, 2008, 128, 164101.	3.0	96
133	Excitation energies in Be: A comparison of multiconfigurational linear response and full configuration interaction calculations. Journal of Chemical Physics, 1986, 85, 6544-6549.	3.0	95
134	Analytic energy gradients for general coupledâ€cluster methods and fourthâ€order manyâ€body perturbation theory. Journal of Chemical Physics, 1986, 85, 5143-5150.	3.0	95
135	Structure and Stability of N6Isomers and Their Spectroscopic Characteristics. Journal of Physical Chemistry A, 2001, 105, 4107-4113.	2.5	95
136	Some aspects of diagrammatic perturbation theory. International Journal of Quantum Chemistry, 1975, 9, 183-198.	2.0	95
137	Time-dependent density functional theory employing optimized effective potentials. Journal of Chemical Physics, 2002, 116, 6468-6481.	3.0	94
138	Highly correlated singleâ€reference studies of the O3 potential surface. I. Effects of high order excitations on the equilibrium structure and harmonic force field of ozone. Journal of Chemical Physics, 1989, 90, 1077-1082.	3.0	92
139	Comparison of MBPT and coupled cluster methods with full CI. II. Polarized basis sets. Journal of Chemical Physics, 1987, 86, 873-881.	3.0	91
140	Critical comparison of single-reference and multireference coupled-cluster methods: Geometry, harmonic frequencies, and excitation energies of N2O2. Journal of Chemical Physics, 2003, 119, 10713-10723.	3.0	91
141	Benchmark Studies on the Building Blocks of DNA. 1. Superiority of Coupled Cluster Methods in Describing the Excited States of Nucleobases in the Franckâ€“Condon Region. Journal of Physical Chemistry A, 2012, 116, 6702-6710.	2.5	91
142	Hyperpolarizabilities of molecules with frequency dependence and electron correlation. Journal of Chemical Physics, 1991, 94, 3665-3669.	3.0	90
143	Can simple localized bond orbitals and coupled cluster methods predict reliable molecular energies?. The Journal of Physical Chemistry, 1985, 89, 2161-2171.	2.9	89
144	Possible Products of the End-On Addition of N3-to N5+and Their Stability. Journal of Physical Chemistry A, 2001, 105, 4096-4106.	2.5	89

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145	The quartic force field of H2O determined by manyâ€body methods. II. Effects of triple excitations. Journal of Chemical Physics, 1987, 87, 6579-6591.	3.0	88
146	Hydrogen pentazole: does it exist?. Journal of the American Chemical Society, 1992, 114, 8302-8303.	13.7	87
147	NMR Spinâ^'Spin Coupling Constants for Hydrogen Bonds of [F(HF)n]-,n= 1â^'4, Clusters. Journal of the American Chemical Society, 2000, 122, 1231-1232.	13.7	86
148	Selection of the reduced virtual space for correlated calculations. An application to the energy and dipole moment of H2O. Chemical Physics Letters, 1989, 159, 148-154.	2.6	85
149	Linear and cyclic isomers of C4. A theoretical study with coupledâ€cluster methods and large basis sets. Journal of Chemical Physics, 1992, 97, 8372-8381.	3.0	85
150	Fifthâ€order manyâ€body perturbation theory for molecular correlation energies. Journal of Chemical Physics, 1989, 90, 7282-7290.	3.0	84
151	Coupled-cluster method for open-shell singlet states. Chemical Physics Letters, 1992, 193, 364-372.	2.6	84
152	Theory and application of MBPT(3) gradients: The density approach. Chemical Physics Letters, 1987, 141, 61-70.	2.6	82
153	Structure and stability of BF3â^—F and AlF3â^—F superhalogens. Chemical Physics Letters, 1998, 292, 289-294.	2.6	82
154	Hilbert space multireference coupledâ€cluster methods. II. A model study on H8. Journal of Chemical Physics, 1992, 97, 4289-4300.	3.0	81
155	Correlation effects in the isomeric cyanides: HNCâ†”HCN, LiNCâ†”gLiCN, and BNCâ†”gBCN. Journal of Chemical Physics, 1980, 72, 986-991.	3.0	80
156	Tailored coupled cluster singles and doubles method applied to calculations on molecular structure and harmonic vibrational frequencies of ozone. Journal of Chemical Physics, 2006, 124, 114311.	3.0	80
157	Molecular applications of the intermediate Hamiltonian Fock-space coupled-cluster method for calculation of excitation energies. Journal of Chemical Physics, 2005, 122, 224110.	3.0	78
158	Dipole polarizability of the fluoride ion with many-body methods. Physical Review A, 1984, 29, 1619-1626.	2.5	77
159	To Multireference or not to Multireference: That is the Question?. International Journal of Molecular Sciences, 2002, 3, 579-603.	4.1	77
160	An application of the equation-of-motion coupled cluster method to the excited states of formaldehyde, acetaldehyde, and acetone. Chemical Physics Letters, 1995, 241, 26-32.	2.6	76
161	Coupled-cluster calculations of Raman intensities and their application to N4 and N5â^'. Chemical Physics Letters, 1999, 314, 381-387.	2.6	76
162	Fock space multireference coupled cluster method with full inclusion of connected triples for excitation energies. Journal of Chemical Physics, 2004, 121, 1670-1675.	3.0	76

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163	Rethinking linearized coupled-cluster theory. Journal of Chemical Physics, 2009, 130, 144112.	3.0	76
164	Multireference Fock-space coupled-cluster and equation-of-motion coupled-cluster theories: The detailed interconnections. Journal of Chemical Physics, 2008, 129, 134105.	3.0	75
165	Analytical MBPT(4) gradients. Chemical Physics Letters, 1988, 153, 490-495.	2.6	74
166	A study of the Be2 potential curve using the full (CCSDT) coupledâ€cluster method: The importance of T4 clusters. Journal of Chemical Physics, 1988, 88, 5974-5976.	3.0	74
167	High-order determinantal equation-of-motion coupled-cluster calculations for ionized and electron-attached states. Chemical Physics Letters, 2000, 328, 459-468.	2.6	74
168	Increasing the applicability of density functional theory. II. Correlation potentials from the random phase approximation and beyond. Journal of Chemical Physics, 2012, 136, 044105.	3.0	74
169	Increasing the applicability of DFT I: Non-variational correlation corrections from Hartreeâ€“Fock DFT for predicting transition states. Chemical Physics Letters, 2012, 524, 10-15.	2.6	72
170	Optimized virtual orbital space for highâ€level correlated calculations. II. Electric properties. Journal of Chemical Physics, 1988, 88, 5749-5758.	3.0	71
171	A benchmark coupled-cluster single, double, and triple excitation (CCSDT) study of the structure and harmonic vibrational frequencies of the ozone molecule. Chemical Physics Letters, 1991, 178, 471-474.	2.6	71
172	Structure and stability of the AlX and AlXâ‾ species. Journal of Chemical Physics, 1999, 110, 2928-2935.	3.0	70
173	Singular value decomposition approach for the approximate coupled-cluster method. Journal of Chemical Physics, 2003, 119, 7756-7762.	3.0	70
174	Ab initio calculations on the energy of activation and tunneling in the automerization of cyclobutadiene. Journal of Chemical Physics, 1988, 89, 3008-3015.	3.0	69
175	Analytic energy derivatives in manyâ€body methods. II. Second derivatives. Journal of Chemical Physics, 1989, 90, 1767-1773.	3.0	69
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