Henrik Koch

List of Publications by Year
in descending order

Version: 2024-02-01

159 papers	17,511 citations	31902 53 h-index	12910 131 g-index
168 all docs	168 docs citations	168 times ranked	7581 citing authors

#	Article	IF	Citations
1	The effect of midbond functions on interaction energies computed using <scp>MP2</scp> and <scp>CCSD</scp>(T). Journal of Computational Chemistry, 2022, 43, 121-131.	1.5	4
2	Excited state absorption of DNA bases in the gas phase and in chloroform solution: a comparative quantum mechanical study. Physical Chemistry Chemical Physics, 2022, 24, 4987-5000.	1.3	7
3	Simulating weak-field attosecond processes with a Lanczos reduced basis approach to time-dependent equation-of-motion coupled-cluster theory. Physical Review A, 2022, 105, .	1.0	14
4	Multi-electron excitation contributions towards primary and satellite states in the photoelectron spectrum. Physical Chemistry Chemical Physics, 2022, 24, 8329-8343.	1.3	7
5	Molecular orbital theory in cavity QED environments. Nature Communications, 2022, 13, 1368.	5.8	27
6	Efficient implementation of molecular CCSD gradients with Cholesky-decomposed electron repulsion integrals. Journal of Chemical Physics, 2022, 156, .	1.2	7
7	On the characteristic features of ionization in QED environments. Journal of Chemical Physics, 2022, 156, .	1.2	15
8	New and Efficient Implementation of CC3. Journal of Chemical Theory and Computation, 2021, 17, 117-126.	2.3	27
9	Biorthonormal Formalism for Nonadiabatic Coupled Cluster Dynamics. Journal of Chemical Theory and Computation, 2021, 17, 127-138.	2.3	3
10	Energy-Based Molecular Orbital Localization in a Specific Spatial Region. Journal of Chemical Theory and Computation, 2021, 17, 139-150.	2.3	14
11	Multilevel CC2 and CCSD in Reduced Orbital Spaces: Electronic Excitations in Large Molecular Systems. Journal of Chemical Theory and Computation, 2021, 17, 714-726.	2.3	16
12	Multilevel Density Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 791-803.	2.3	21
13	Excited-State Absorption of Uracil in the Gas Phase: Mapping the Main Decay Paths by Different Electronic Structure Methods. Journal of Chemical Theory and Computation, 2021, 17, 1638-1652.	2.3	15
14	Intermolecular interactions in optical cavities: An ab initio QED study. Journal of Chemical Physics, 2021, 154, 094113.	1.2	81
15	Equation-of-motion coupled-cluster method with double electron-attaching operators: Theory, implementation, and benchmarks. Journal of Chemical Physics, 2021, 154, 114115.	1.2	17
16	Describing ground and excited state potential energy surfaces for molecular photoswitches using coupled cluster models. Journal of Computational Chemistry, 2021, 42, 1419-1429.	1.5	4
17	Strong Coupling between Localized Surface Plasmons and Molecules by Coupled Cluster Theory. Nano Letters, 2021, 21, 6664-6670.	4.5	32
18	Transient resonant Augerâ€“Meitner spectra of photoexcited thymine. Faraday Discussions, 2021, 228, 555-570.	1.6	11

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19	Combining multilevel Hartreeâ€“Fock and multilevel coupled cluster approaches with molecular mechanics: a study of electronic excitations in solutions. Physical Chemistry Chemical Physics, 2021, 23, 4413-4425.	1.3	12
20	Predictions of Pre-edge Features in Time-Resolved Near-Edge X-ray Absorption Fine Structure Spectroscopy from Holeâ€“Hole Tammâ€“Dancoff-Approximated Density Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 7120-7133.	2.3	3
21	Linear-Scaling Implementation of Multilevel Hartreeâ€“Fock Theory. Journal of Chemical Theory and Computation, 2021, 17, 7416-7427.	2.3	4
22	Multilevel CC2 and CCSD Methods with Correlated Natural Transition Orbitals. Journal of Chemical Theory and Computation, 2020, 16, 179-189.	2.3	27
23	Accelerated multimodel Newton-type algorithms for faster convergence of ground and excited state coupled cluster equations. Journal of Chemical Physics, 2020, 153, 014104.	1.2	6
24	Equation-of-Motion MLCCSD and CCSD-in-HF Oscillator Strengths and Their Application to Core Excitations. Journal of Chemical Theory and Computation, 2020, 16, 6869-6879.	2.3	17
25	Time-dependent coupled-cluster theory for ultrafast transient-absorption spectroscopy. Physical Review A, 2020, 102, .	1.0	20
26	Coupled Cluster Theory for Molecular Polaritons: Changing Ground and Excited States. Physical Review X, 2020, 10, .	2.8	102
27	e T 1.0: An open source electronic structure program with emphasis on coupled cluster and multilevel methods. Journal of Chemical Physics, 2020, 152, 184103.	1.2	68
28	Accurate Description of Photoionization Dynamical Parameters. Journal of Physical Chemistry Letters, 2020, 11, 5330-5337.	2.1	26
29	An efficient algorithm for Cholesky decomposition of electron repulsion integrals. Journal of Chemical Physics, 2019, 150, 194112.	1.2	46
30	Observation of Ultrafast Intersystem Crossing in Thymine by Extreme Ultraviolet Time-Resolved Photoelectron Spectroscopy. Journal of Physical Chemistry A, 2019, 123, 6897-6903.	1.1	29
31	Spin adapted implementation of EOM-CCSD for triplet excited states: Probing intersystem crossings of acetylacetone at the carbon and oxygen K-edges. Journal of Chemical Physics, 2019, 151, 144107.	1.2	12
32	X-ray and UV Spectra of Glycine within Coupled Cluster Linear Response Theory. Journal of Physical Chemistry A, 2019, 123, 9701-9711.	1.1	14
33	An Orbital Invariant Similarity Constrained Coupled Cluster Model. Journal of Chemical Theory and Computation, 2019, 15, 5386-5397.	2.3	7
34	An analysis of the performance of coupled cluster methods for K-edge core excitations and ionizations using standard basis sets. Advances in Quantum Chemistry, 2019, 79, 241-261.	0.4	30
35	A theoretical and experimental benchmark study of core-excited states in nitrogen. Journal of Chemical Physics, 2018, 148, 064106.	1.2	27
36	Large-Scale Electron Correlation Calculations: Rank-Reduced Full Configuration Interaction. Journal of Chemical Theory and Computation, 2018, 14, 4139-4150.	2.3	23

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37	Probing ultrafast Ï€Ï€*/nÏ€* internal conversion in organic chromophores via K-edge resonant absorption. Nature Communications, 2017, 8, 29.	5.8	144
38	Solvent Effects on Optical Rotation: On the Balance between Hydrogen Bonding and Shifts in Dihedral Angles. Journal of Physical Chemistry A, 2017, 121, 4765-4777.	1.1	10
39	Density-Based Multilevel Hartreeâ€“Fock Model. Journal of Chemical Theory and Computation, 2017, 13, 5282-5290.	2.3	30
40	Resolving the Notorious Case of Conical Intersections for Coupled Cluster Dynamics. Journal of Physical Chemistry Letters, 2017, 8, 4801-4807.	2.1	28
41	Tautomerization of Thymine Using Ultraviolet Light. Langmuir, 2017, 33, 9666-9672.	1.6	4
42	Crossing conditions in coupled cluster theory. Journal of Chemical Physics, 2017, 147, 164105.	1.2	40
43	Correlated natural transition orbitals for core excitation energies in multilevel coupled cluster models. Journal of Chemical Physics, 2017, 146, 144109.	1.2	31
44	Potential Energy Surfaces and Charge Transfer of PAHâ€Sodiumâ€PAH Complexes. ChemPhysChem, 2016, 17, 2908-2915.	1.0	3
45	The multilevel CC3 coupled cluster model. Journal of Chemical Physics, 2016, 145, 044111.	1.2	37
46	Optical Rotation Calculations for a Set of Pyrrole Compounds. Journal of Physical Chemistry A, 2016, 120, 7351-7360.	1.1	17
47	Optical Rotation Calculations for Fluorinated Alcohols, Amines, Amides, and Esters. Journal of Physical Chemistry A, 2016, 120, 7973-7986.	1.1	9
48	A ReaxFF force field for sodium intrusion in graphitic cathodes. Physical Chemistry Chemical Physics, 2016, 18, 31431-31440.	1.3	18
49	Chemically accurate energy barriers of small gas molecules moving through hexagonal water rings. Physical Chemistry Chemical Physics, 2016, 18, 17831-17835.	1.3	5
50	Near-Edge X-ray Absorption Fine Structure within Multilevel Coupled Cluster Theory. Journal of Chemical Theory and Computation, 2016, 12, 2633-2643.	2.3	35
51	Optical Rotation from Coupled Cluster and Density Functional Theory: The Role of Basis Set Convergence. Journal of Chemical Theory and Computation, 2016, 12, 535-548.	2.3	21
52	Transient NEXAFS Spectroscopy at the Oxygen Edge: Pinning Down Ï€Ï€*/nÏ€* Internal Conversion. , 2016, , .		1
53	Communication: X-ray absorption spectra and core-ionization potentials within a core-valence separated coupled cluster framework. Journal of Chemical Physics, 2015, 143, 181103.	1.2	162
54	Density Functional Theory Study on the Interactions of Metal Ions with Long Chain Deprotonated Carboxylic Acids. Journal of Physical Chemistry A, 2015, 119, 10195-10203.	1.1	33

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55	A benchmark study of electronic excitation energies, transition moments, and excited-state energy gradients on the nicotine molecule. Journal of Chemical Physics, 2014, 141, 224114.	1.2	23
56	Multi-level coupled cluster theory. Journal of Chemical Physics, 2014, 141, 224105.	1.2	45
57	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	6.2	1,166
58	Assessment of density functionals for van der Waals complexes of sodium and benzene. Molecular Physics, 2013, 111, 1211-1218.	0.8	5
59	The extended CC2 model ECC2. Molecular Physics, 2013, 111, 1109-1118.	0.8	19
60	The CCSD(T) model with Cholesky decomposition of orbital energy denominators. International Journal of Quantum Chemistry, 2011, 111, 349-355.	1.0	11
61	Cholesky Decomposition Techniques in Electronic Structure Theory. Challenges and Advances in Computational Chemistry and Physics, 2011, , 301-343.	0.6	71
62	Cholesky decomposition-based definition of atomic subsystems in electronic structure calculations. Journal of Chemical Physics, 2010, 132, 204105.	1.2	22
63	Coupled cluster response theory in parameter subspaces. International Journal of Quantum Chemistry, 2009, 109, 708-716.	1.0	1
64	The Benzeneâ˜Argon Ground-State Intermolecular Potential Energy Surface Revisited. Journal of Physical Chemistry A, 2009, 113, 5212-5216.	1.1	22
65	Method specific Cholesky decomposition: Coulomb and exchange energies. Journal of Chemical Physics, 2008, 129, 134107.	1.2	54
66	Variation of polarizability in the [4n + 2] annulene series: from [22]- to [66]-annulene. Physical Chemistry Chemical Physics, 2008, 10, 361-365.	1.3	15
67	Accurate ab initio density fitting for multiconfigurational self-consistent field methods. Journal of Chemical Physics, 2008, 129, 024113.	1.2	161
68	Basis set limits of the second order MÃ¸ller-Plesset correlation energies of water, methane, acetylene, ethylene, and benzene. Journal of Chemical Physics, 2007, 127, 144104.	1.2	27
69	Coupled cluster calculations of interaction energies in benzeneâ€“fluorobenzene van der Waals complexes. Chemical Physics Letters, 2007, 441, 332-335.	1.2	14
70	Ab initio potential-energy surface and rovibrational states of the HCNâ€“HCl complex. Journal of Chemical Physics, 2006, 124, 204315.	1.2	13
71	Carbon Nanorings: A Challenge to Theoretical Chemistry. ChemPhysChem, 2006, 7, 2503-2507.	1.0	37
72	Fast noniterative orbital localization for large molecules. Journal of Chemical Physics, 2006, 125, 174101.	1.2	138

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73	Ab Initio Calculation of Optical Rotation in (P)-(+)-[4]Triangulane. Journal of the American Chemical Society, 2005, 127, 1368-1369.	6.6	75
74	Polarizability and optical rotation calculated from the approximate coupled cluster singles and doubles CC2 linear response theory using Cholesky decompositions. Journal of Chemical Physics, 2004, 120, 8887-8897.	1.2	107
75	Polarizabilities of small annulenes from Cholesky CC2 linear response theory. Chemical Physics Letters, 2004, 390, 170-175.	1.2	23
76	Origin invariant calculation of optical rotation without recourse to London orbitals. Chemical Physics Letters, 2004, 393, 319-326.	1.2	156
77	Argon broadening of the 13CO R(0) and R(7) transitions in the fundamental band at temperatures between 80 and 297K: comparison between experiment and theory. Journal of Molecular Spectroscopy, 2003, 222, 131-141.	0.4	21
78	Coupled cluster calculations of the vertical excitation energies of tetracyanoethylene. Journal of Chemical Physics, 2003, 118, 8216-8222.	1.2	12
79	Reduced scaling in electronic structure calculations using Cholesky decompositions. Journal of Chemical Physics, 2003, 118, 9481-9484.	1.2	386
80	Study of the benzeneâ‹…N2 intermolecular potential-energy surface. Journal of Chemical Physics, 2003, 118, 1230-1241.	1.2	16
81	Benzeneâ€“argon triplet intermolecular potential energy surface. Journal of Chemical Physics, 2003, 119, 4762-4767.	1.2	19
82	Computational and experimental investigation of intermolecular states and forces in the benzeneâ€“helium van der Waals complex. Journal of Chemical Physics, 2003, 119, 12956-12964.	1.2	30
83	Theoretical absorption spectrum of the Arâ€“CO van der Waals complex. Journal of Chemical Physics, 2003, 118, 9596-9607.	1.2	9
84	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
85	The effect of intermolecular interactions on the electric properties of helium and argon. III. Quantum statistical calculations of the dielectric second virial coefficients. Journal of Chemical Physics, 2002, 117, 2609-2618.	1.2	60
86	Rovibrational structure of the Arâ€“CO complex based on a novel three-dimensional ab initio potential. Journal of Chemical Physics, 2002, 117, 6562-6572.	1.2	47
87	The heliumâ€“, neonâ€“, and argonâ€“cyclopropane van der Waals complexes: Ab initio ground state intermolecular potential energy surfaces and intermolecular dynamics. Journal of Chemical Physics, 2001, 115, 8431-8439.	1.2	84
88	A coupled cluster calculation of the spectrum of urea. Chemical Physics Letters, 2001, 348, 469-476.	1.2	9
89	Comment on â€œThe importance of high-order correlation effects for the COâ€“CO interaction potentialâ€• [Chem. Phys. Lett. 314 (1999) 326]. Chemical Physics Letters, 2001, 334, 419-423.	1.2	23
90	Gauge invariant coupled cluster response theory using optimized nonorthogonal orbitals. Journal of Chemical Physics, 2001, 114, 6983-6993.	1.2	82

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91	Propagator Calculations of Electronic Spectra of Photochromic Spirooxazines. Molecular Crystals and Liquid Crystals, 2000, 345, 89-94.	0.3	1
92	Size-intensive decomposition of orbital energy denominators. Journal of Chemical Physics, 2000, 113, 508-513.	1.2	43
93	Atomic integral driven second order polarization propagator calculations of the excitation spectra of naphthalene and anthracene. Journal of Chemical Physics, 2000, 112, 4173-4185.	1.2	131
94	Theoretical electronic absorption and natural circular dichroism spectra of (â^')-trans-cyclooctene. Journal of Chemical Physics, 2000, 112, 2139-2147.	1.2	26
95	Coupled-cluster calculations on ferrocene and its protonated derivatives: Towards the final word on the mechanism of protonation of ferrocene?. Journal of Chemical Physics, 2000, 113, 8009-8014.	1.2	25
96	The effect of intermolecular interactions on the electric properties of helium and argon. I. Ab initio calculation of the interaction induced polarizability and hyperpolarizability in He2 and Ar2. Journal of Chemical Physics, 1999, 111, 10099-10107.	1.2	75
97	Gauge invariant coupled cluster response theory. Journal of Chemical Physics, 1999, 110, 8318-8327.	1.2	96
98	Coupled cluster response calculation of natural chiroptical spectra. Journal of Chemical Physics, 1999, 110, 2883-2892.	1.2	75
99	The effect of intermolecular interactions on the electric properties of helium and argon. II. The dielectric, refractivity, Kerr, and hyperpolarizability second virial coefficients. Journal of Chemical Physics, 1999, 111, 10108-10118.	1.2	48
100	Ab initiocalculation of the frequency-dependent interaction induced hyperpolarizability of Ar2. Journal of Chemical Physics, 1999, 110, 2872-2882.	1.2	46
101	Accurate intermolecular ground state potential of the Arâ€"N2 complex. Journal of Chemical Physics, 1999, 110, 8525-8532.	1.2	35
102	Ground state benzeneâ€"argon intermolecular potential energy surface. Journal of Chemical Physics, 1999, 111, 198-204.	1.2	86
103	Benzene-argon S1 intermolecular potential energy surface. Journal of Chemical Physics, 1999, 111, 5922-5928.	1.2	44
104	A second-order doubles correction to excitation energies in the random-phase approximation. Chemical Physics Letters, 1998, 284, 47-55.	1.2	39
105	The Hartreeâ€"Fock magnetizability of C60. Chemical Physics Letters, 1998, 285, 205-209.	1.2	16
106	Basis-set convergence in correlated calculations on Ne, N2, and H2O. Chemical Physics Letters, 1998, 286, 243-252.	1.2	1,989
107	Gauge invariance of the coupled cluster oscillator strength. Chemical Physics Letters, 1998, 293, 251-260.	1.2	36
108	The vibrational and temperature dependence of the indirect nuclear spinâ€"spin coupling constants of the oxonium (H3O+) and hydroxyl (OHâ^) ions. Chemical Physics, 1998, 238, 385-399.	0.9	49

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109	Accurate ab initio rovibronic spectrum of the Xâ€‰1Î£g+ and Bâ€‰1Î£u+ states in Ar2. Journal of Chemical Physics, 1998, 109, 10255-10262.	1.2	31
110	On the time-dependent Lagrangian approach in quantum chemistry. Journal of Chemical Physics, 1998, 108, 5194-5204.	1.2	24
111	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
112	The Cottonâ€“Mouton effect of liquid water. Part II: The semi-continuum model. Journal of Chemical Physics, 1998, 108, 599-603.	1.2	20
113	The benzeneâ€“argon complex: A ground and excited state ab initio study. Journal of Chemical Physics, 1998, 108, 2784-2790.	1.2	144
114	C24: Ring or fullerene?. Journal of Chemical Physics, 1998, 108, 3213-3217.	1.2	31
115	Comment on â€œFrequency-dependent equation-of-motion coupled cluster hyperpolarizabilities: Resolution of the discrepancy between theory and experiment for HF?â€•[J. Chem. Phys. 107, 10823 (1997)]. Journal of Chemical Physics, 1998, 109, 3293-3295.	1.2	11
116	Comment on â€œResponse to â€˜Comment on â€œFrequency-dependent equation-of-motion coupled cluster hyperpolarizabilities: Resolution of the discrepancy between theory and experiment for HF?â€â€‰â€™â€‰â€•[J. Chem. Phys. 109, 9201 (1998)]. Journal of Chemical Physics, 1998, 109, 9204-9204.	1.2	2
117	The CC3 model: An iterative coupled cluster approach including connected triples. Journal of Chemical Physics, 1997, 106, 1808-1818.	1.2	412
118	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
119	Basis-set convergence of correlated calculations on water. Journal of Chemical Physics, 1997, 106, 9639-9646.	1.2	2,197
120	Coupled cluster response functions revisited. Journal of Chemical Physics, 1997, 106, 8059-8072.	1.2	120
121	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
122	Multiple basis sets in calculations of triples corrections in coupled-cluster theory. Theoretical Chemistry Accounts, 1997, 97, 164-176.	0.5	82
123	Frequency-dependent first hyperpolarizabilities using coupled cluster quadratic response theory. Chemical Physics Letters, 1997, 269, 428-434.	1.2	125
124	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.	1.2	260
125	Surprising cases of divergent behavior in Mo/llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 1996, 105, 5082-5090.	1.2	192
126	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

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127	Efficient parallel implementation of response theory: Calculations of the second hyperpolarizability of polyacenes. Chemical Physics Letters, 1996, 253, 1-7.	1.2	47
128	Dynamic CCSD polarisabilities of CHF3 and CHCl3. Chemical Physics Letters, 1996, 253, 373-376.	1.2	13
129	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
130	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
131	Integral direct calculation of CC2 excitation energies: singlet excited states of benzene. Chemical Physics Letters, 1996, 263, 530-539.	1.2	53
132	Perturbative triple excitation corrections to coupled cluster singles and doubles excitation energies. Journal of Chemical Physics, 1996, 105, 1451-1459.	1.2	211
133	The molecular structure of ferrocene. Journal of Chemical Physics, 1996, 104, 9528-9530.	1.2	98
134	The integralâ€direct coupled cluster singles and doubles model. Journal of Chemical Physics, 1996, 104, 4157-4165.	1.2	154
135	The second-order approximate coupled cluster singles and doubles model CC2. Chemical Physics Letters, 1995, 243, 409-418.	1.2	1,564
136	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
137	Random-phase calculations of frequency-dependent polarizabilities and hyperpolarizabilities of long polyene chains. Physical Review B, 1995, 51, 14949-14957.	1.1	31
138	SCF calculations of the NMR shielding tensor for the ethylenic carbon atom in C3Cl4. Molecular Physics, 1995, 85, 671-673.	0.8	6
139	Response functions in the CC3 iterative triple excitation model. Journal of Chemical Physics, 1995, 103, 7429-7441.	1.2	498
140	Static polarizabilities and dipole moment derivatives for the closed shell coupled cluster singles and doubles wave function. Journal of Chemical Physics, 1994, 101, 4956-4963.	1.2	18
141	Calculation of sizeâ€intensive transition moments from the coupled cluster singles and doubles linear response function. Journal of Chemical Physics, 1994, 100, 4393-4400.	1.2	217
142	Brueckner coupled cluster response functions. International Journal of Quantum Chemistry, 1994, 49, 835-848.	1.0	21
143	Calculation of frequency-dependent polarizabilities using coupled-cluster response theory. Chemical Physics Letters, 1994, 219, 30-35.	1.2	115
144	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

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145	Comparison of coupled-cluster and Brueckner coupled-cluster calculations of molecular properties. Chemical Physics Letters, 1993, 211, 94-100.	1.2	67
146	Linear superposition of optimized non-orthogonal Slater determinants for singlet states. Chemical Physics Letters, 1993, 212, 193-200.	1.2	21
147	Quartic coupled cluster force fields for the diazene isomers. Chemical Physics Letters, 1993, 215, 576-581.	1.2	10
148	Large scale random phase calculations for direct self-consistent field wavefunctions. Chemical Physics, 1993, 172, 13-20.	0.9	29
149	Frequency dependent hyperpolarizabilities of polyynes. Journal of Chemical Physics, 1993, 98, 7229-7235.	1.2	31
150	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
151	A variational matrix decomposition applied to full configuration-interaction calculations. Chemical Physics Letters, 1992, 198, 51-58.	1.2	6
152	Analytical calculation of full configuration interaction response properties: Application to Be. Journal of Chemical Physics, 1991, 95, 7479-7485.	1.2	53
153	Branching ratios for the dissociative decay of tripletH2. Physical Review A, 1991, 44, 4171-4179.	1.0	30
154	Coupled cluster response functions. Journal of Chemical Physics, 1990, 93, 3333-3344.	1.2	975
155	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
156	Determination of the transition dipole moment Î¼â†'b(R) in H2 from the measurement of vibrational wave functions. Journal of Chemical Physics, 1990, 93, 3887-3890.	1.2	6
157	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
158	The infrared spectrum of water. Basis set dependence at the single and double excitation coupled cluster (CCSD) level of theory. Chemical Physics Letters, 1988, 149, 118-122.	1.2	13
159	Direct iterative RPA calculations. Applications to ethylene, benzene and cytosine. Chemical Physics, 1988, 119, 297-306.	0.9	37