Henrik Koch

List of Publications by Year
in descending order

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	Basis-set convergence of correlated calculations on water. Journal of Chemical Physics, 1997, 106, 9639-9646.	1.2	2,197
2	Basis-set convergence in correlated calculations on Ne, N2, and H2O. Chemical Physics Letters, 1998, 286, 243-252.	1.2	1,989
3	The second-order approximate coupled cluster singles and doubles model CC2. Chemical Physics Letters, 1995, 243, 409-418.	1.2	1,564
4	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	6.2	1,166
5	Coupled cluster response functions. Journal of Chemical Physics, 1990, 93, 3333-3344.	1.2	975
6	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
7	Response functions in the CC3 iterative triple excitation model. Journal of Chemical Physics, 1995, 103, 7429-7441.	1.2	498
8	The CC3 model: An iterative coupled cluster approach including connected triples. Journal of Chemical Physics, 1997, 106, 1808-1818.	1.2	412
9	Reduced scaling in electronic structure calculations using Cholesky decompositions. Journal of Chemical Physics, 2003, 118, 9481-9484.	1.2	386
10	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
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	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
13	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
14	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
15	Perturbative triple excitation corrections to coupled cluster singles and doubles excitation energies. Journal of Chemical Physics, 1996, 105, 1451-1459.	1.2	211
16	Surprising cases of divergent behavior in Mo/llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 1996, 105, 5082-5090.	1.2	192
17	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
18	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

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19	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
20	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
21	Accurate <i>ab initio</i> density fitting for multiconfigurational self-consistent field methods. Journal of Chemical Physics, 2008, 129, 024113.	1.2	161
22	Origin invariant calculation of optical rotation without recourse to London orbitals. Chemical Physics Letters, 2004, 393, 319-326.	1.2	156
23	The integralâ€direct coupled cluster singles and doubles model. Journal of Chemical Physics, 1996, 104, 4157-4165.	1.2	154
24	The benzeneâ€“argon complex: A ground and excited state ab initio study. Journal of Chemical Physics, 1998, 108, 2784-2790.	1.2	144
25	Probing ultrafast Ï€Ï€*/nÏ€* internal conversion in organic chromophores via K-edge resonant absorption. Nature Communications, 2017, 8, 29.	5.8	144
26	Fast noniterative orbital localization for large molecules. Journal of Chemical Physics, 2006, 125, 174101.	1.2	138
27	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
28	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
29	Frequency-dependent first hyperpolarizabilities using coupled cluster quadratic response theory. Chemical Physics Letters, 1997, 269, 428-434.	1.2	125
30	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
31	Coupled cluster response functions revisited. Journal of Chemical Physics, 1997, 106, 8059-8072.	1.2	120
32	Calculation of frequency-dependent polarizabilities using coupled-cluster response theory. Chemical Physics Letters, 1994, 219, 30-35.	1.2	115
33	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
34	Coupled Cluster Theory for Molecular Polaritons: Changing Ground and Excited States. Physical Review X, 2020, 10, .	2.8	102
35	The molecular structure of ferrocene. Journal of Chemical Physics, 1996, 104, 9528-9530.	1.2	98
36	Gauge invariant coupled cluster response theory. Journal of Chemical Physics, 1999, 110, 8318-8327.	1.2	96

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37	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
38	Ground state benzeneâ€“argon intermolecular potential energy surface. Journal of Chemical Physics, 1999, 111, 198-204.	1.2	86
39	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
40	Multiple basis sets in calculations of triples corrections in coupled-cluster theory. Theoretical Chemistry Accounts, 1997, 97, 164-176.	0.5	82
41	Gauge invariant coupled cluster response theory using optimized nonorthogonal orbitals. Journal of Chemical Physics, 2001, 114, 6983-6993.	1.2	82
42	Intermolecular interactions in optical cavities: An <i>ab initio</i> QED study. Journal of Chemical Physics, 2021, 154, 094113.	1.2	81
43	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
44	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
45	Coupled cluster response calculation of natural chiroptical spectra. Journal of Chemical Physics, 1999, 110, 2883-2892.	1.2	75
46	Ab Initio Calculation of Optical Rotation in (P)-(+)-[4]Triangulane. Journal of the American Chemical Society, 2005, 127, 1368-1369.	6.6	75
47	Cholesky Decomposition Techniques in Electronic Structure Theory. Challenges and Advances in Computational Chemistry and Physics, 2011, , 301-343.	0.6	71
48	<i>e</i> <i>T</i> 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
49	Comparison of coupled-cluster and Brueckner coupled-cluster calculations of molecular properties. Chemical Physics Letters, 1993, 211, 94-100.	1.2	67
50	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
51	Method specific Cholesky decomposition: Coulomb and exchange energies. Journal of Chemical Physics, 2008, 129, 134107.	1.2	54
52	Analytical calculation of full configuration interaction response properties: Application to Be. Journal of Chemical Physics, 1991, 95, 7479-7485.	1.2	53
53	Integral direct calculation of CC2 excitation energies: singlet excited states of benzene. Chemical Physics Letters, 1996, 263, 530-539.	1.2	53
54	The vibrational and temperature dependence of the indirect nuclear spinâ€“spin coupling constants of the oxonium (H3O+) and hydroxyl (OHâˆ’) ions. Chemical Physics, 1998, 238, 385-399.	0.9	49

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55	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
56	Efficient parallel implementation of response theory: Calculations of the second hyperpolarizability of polyacenes. Chemical Physics Letters, 1996, 253, 1-7.	1.2	47
57	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
58	Ab initiocalculation of the frequency-dependent interaction induced hyperpolarizability of Ar2. Journal of Chemical Physics, 1999, 110, 2872-2882.	1.2	46
59	An efficient algorithm for Cholesky decomposition of electron repulsion integrals. Journal of Chemical Physics, 2019, 150, 194112.	1.2	46
60	Multi-level coupled cluster theory. Journal of Chemical Physics, 2014, 141, 224105.	1.2	45
61	Benzene-argon S1 intermolecular potential energy surface. Journal of Chemical Physics, 1999, 111, 5922-5928.	1.2	44
62	Size-intensive decomposition of orbital energy denominators. Journal of Chemical Physics, 2000, 113, 508-513.	1.2	43
63	Crossing conditions in coupled cluster theory. Journal of Chemical Physics, 2017, 147, 164105.	1.2	40
64	A second-order doubles correction to excitation energies in the random-phase approximation. Chemical Physics Letters, 1998, 284, 47-55.	1.2	39
65	Direct iterative RPA calculations. Applications to ethylene, benzene and cytosine. Chemical Physics, 1988, 119, 297-306.	0.9	37
66	Carbon Nanorings: A Challenge to Theoretical Chemistry. ChemPhysChem, 2006, 7, 2503-2507.	1.0	37
67	The multilevel CC3 coupled cluster model. Journal of Chemical Physics, 2016, 145, 044111.	1.2	37
68	Gauge invariance of the coupled cluster oscillator strength. Chemical Physics Letters, 1998, 293, 251-260.	1.2	36
69	Accurate intermolecular ground state potential of the Arâ€"N2 complex. Journal of Chemical Physics, 1999, 110, 8525-8532.	1.2	35
70	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
71	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
72	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

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73	Strong Coupling between Localized Surface Plasmons and Molecules by Coupled Cluster Theory. Nano Letters, 2021, 21, 6664-6670.	4.5	32
74	Frequency dependent hyperpolarizabilities of polyynes. Journal of Chemical Physics, 1993, 98, 7229-7235.	1.2	31
75	Random-phase calculations of frequency-dependent polarizabilities and hyperpolarizabilities of long polyene chains. Physical Review B, 1995, 51, 14949-14957.	1.1	31
76	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
77	C24: Ring or fullerene?. Journal of Chemical Physics, 1998, 108, 3213-3217.	1.2	31
78	Correlated natural transition orbitals for core excitation energies in multilevel coupled cluster models. Journal of Chemical Physics, 2017, 146, 144109.	1.2	31
79	Branching ratios for the dissociative decay of tripletH2. Physical Review A, 1991, 44, 4171-4179.	1.0	30
80	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
81	Density-Based Multilevel Hartreeâ€"Fock Model. Journal of Chemical Theory and Computation, 2017, 13, 5282-5290.	2.3	30
82	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
83	Large scale random phase calculations for direct self-consistent field wavefunctions. Chemical Physics, 1993, 172, 13-20.	0.9	29
84	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
85	Resolving the Notorious Case of Conical Intersections for Coupled Cluster Dynamics. Journal of Physical Chemistry Letters, 2017, 8, 4801-4807.	2.1	28
86	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
87	A theoretical and experimental benchmark study of core-excited states in nitrogen. Journal of Chemical Physics, 2018, 148, 064106.	1.2	27
88	Multilevel CC2 and CCSD Methods with Correlated Natural Transition Orbitals. Journal of Chemical Theory and Computation, 2020, 16, 179-189.	2.3	27
89	New and Efficient Implementation of CC3. Journal of Chemical Theory and Computation, 2021, 17, 117-126.	2.3	27
90	Molecular orbital theory in cavity QED environments. Nature Communications, 2022, 13, 1368.	5.8	27

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91	Theoretical electronic absorption and natural circular dichroism spectra of (â^')-trans-cyclooctene. Journal of Chemical Physics, 2000, 112, 2139-2147.	1.2	26
92	Accurate Description of Photoionization Dynamical Parameters. Journal of Physical Chemistry Letters, 2020, 11, 5330-5337.	2.1	26
93	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
94	On the time-dependent Lagrangian approach in quantum chemistry. Journal of Chemical Physics, 1998, 108, 5194-5204.	1.2	24
95	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
96	Polarizabilities of small annulenes from Cholesky CC2 linear response theory. Chemical Physics Letters, 2004, 390, 170-175.	1.2	23
97	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
98	Large-Scale Electron Correlation Calculations: Rank-Reduced Full Configuration Interaction. Journal of Chemical Theory and Computation, 2018, 14, 4139-4150.	2.3	23
99	The Benzeneâ^'Argon Ground-State Intermolecular Potential Energy Surface Revisited. Journal of Physical Chemistry A, 2009, 113, 5212-5216.	1.1	22
100	Cholesky decomposition-based definition of atomic subsystems in electronic structure calculations. Journal of Chemical Physics, 2010, 132, 204105.	1.2	22
101	Linear superposition of optimized non-orthogonal Slater determinants for singlet states. Chemical Physics Letters, 1993, 212, 193-200.	1.2	21
102	Brueckner coupled cluster response functions. International Journal of Quantum Chemistry, 1994, 49, 835-848.	1.0	21
103	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
104	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
105	Multilevel Density Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 791-803.	2.3	21
106	The Cottonâ€"Mouton effect of liquid water. Part II: The semi-continuum model. Journal of Chemical Physics, 1998, 108, 599-603.	1.2	20
107	Time-dependent coupled-cluster theory for ultrafast transient-absorption spectroscopy. Physical Review A, 2020, 102, .	1.0	20
108	Benzeneâ€"argon triplet intermolecular potential energy surface. Journal of Chemical Physics, 2003, 119, 4762-4767.	1.2	19

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109	The extended CC2 model ECC2. Molecular Physics, 2013, 111, 1109-1118.	0.8	19
110	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
111	A ReaxFF force field for sodium intrusion in graphitic cathodes. Physical Chemistry Chemical Physics, 2016, 18, 31431-31440.	1.3	18
112	Optical Rotation Calculations for a Set of Pyrrole Compounds. Journal of Physical Chemistry A, 2016, 120, 7351-7360.	1.1	17
113	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
114	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
115	The Hartreeâ€“Fock magnetizability of C60. Chemical Physics Letters, 1998, 285, 205-209.	1.2	16
116	Study of the benzeneâ‹…N2 intermolecular potential-energy surface. Journal of Chemical Physics, 2003, 118, 1230-1241.	1.2	16
117	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
118	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
119	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
120	On the characteristic features of ionization in QED environments. Journal of Chemical Physics, 2022, 156, .	1.2	15
121	Coupled cluster calculations of interaction energies in benzeneâ€“fluorobenzene van der Waals complexes. Chemical Physics Letters, 2007, 441, 332-335.	1.2	14
122	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
123	Energy-Based Molecular Orbital Localization in a Specific Spatial Region. Journal of Chemical Theory and Computation, 2021, 17, 139-150.	2.3	14
124	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
125	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
126	Dynamic CCSD polarisabilities of CHF3 and CHCl3. Chemical Physics Letters, 1996, 253, 373-376.	1.2	13

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127	Ab initio potential-energy surface and rovibrational states of the HCNâ€“HCl complex. Journal of Chemical Physics, 2006, 124, 204315.	1.2	13
128	Coupled cluster calculations of the vertical excitation energies of tetracyanoethylene. Journal of Chemical Physics, 2003, 118, 8216-8222.	1.2	12
129	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
130	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
131	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
132	The CCSD(T) model with Cholesky decomposition of orbital energy denominators. International Journal of Quantum Chemistry, 2011, 111, 349-355.	1.0	11
133	Transient resonant Augerâ€“Meitner spectra of photoexcited thymine. Faraday Discussions, 2021, 228, 555-570.	1.6	11
134	Quartic coupled cluster force fields for the diazene isomers. Chemical Physics Letters, 1993, 215, 576-581.	1.2	10
135	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
136	A coupled cluster calculation of the spectrum of urea. Chemical Physics Letters, 2001, 348, 469-476.	1.2	9
137	Theoretical absorption spectrum of the Arâ€“CO van der Waals complex. Journal of Chemical Physics, 2003, 118, 9596-9607.	1.2	9
138	Optical Rotation Calculations for Fluorinated Alcohols, Amines, Amides, and Esters. Journal of Physical Chemistry A, 2016, 120, 7973-7986.	1.1	9
139	An Orbital Invariant Similarity Constrained Coupled Cluster Model. Journal of Chemical Theory and Computation, 2019, 15, 5386-5397.	2.3	7
140	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
141	Multi-electron excitation contributions towards primary and satellite states in the photoelectron spectrum. Physical Chemistry Chemical Physics, 2022, 24, 8329-8343.	1.3	7
142	Efficient implementation of molecular CCSD gradients with Cholesky-decomposed electron repulsion integrals. Journal of Chemical Physics, 2022, 156, .	1.2	7
143	Determination of the transition dipole moment Î¼iâ†’b(R) in H2 from the measurement of vibrational wave functions. Journal of Chemical Physics, 1990, 93, 3887-3890.	1.2	6
144	A variational matrix decomposition applied to full configuration-interaction calculations. Chemical Physics Letters, 1992, 198, 51-58.	1.2	6

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145	SCF calculations of the NMR shielding tensor for the ethylenic carbon atom in C3Cl4. Molecular Physics, 1995, 85, 671-673.	0.8	6
146	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
147	Assessment of density functionals for van der Waals complexes of sodium and benzene. Molecular Physics, 2013, 111, 1211-1218.	0.8	5
148	Chemically accurate energy barriers of small gas molecules moving through hexagonal water rings. Physical Chemistry Chemical Physics, 2016, 18, 17831-17835.	1.3	5
149	Tautomerization of Thymine Using Ultraviolet Light. Langmuir, 2017, 33, 9666-9672.	1.6	4
150	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
151	Linear-Scaling Implementation of Multilevel Hartreeâ€"Fock Theory. Journal of Chemical Theory and Computation, 2021, 17, 7416-7427.	2.3	4
152	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
153	Potential Energy Surfaces and Charge Transfer of PAHâ€Sodiumâ€PAH Complexes. ChemPhysChem, 2016, 17, 2908-2915.	1.0	3
154	Biorthonormal Formalism for Nonadiabatic Coupled Cluster Dynamics. Journal of Chemical Theory and Computation, 2021, 17, 127-138.	2.3	3
155	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
156	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
157	Propagator Calculations of Electronic Spectra of Photochromic Spirooxazines. Molecular Crystals and Liquid Crystals, 2000, 345, 89-94.	0.3	1
158	Coupled cluster response theory in parameter subspaces. International Journal of Quantum Chemistry, 2009, 109, 708-716.	1.0	1
159	Transient NEXAFS Spectroscopy at the Oxygen Edge: Pinning Down Ï€Ï€*/nÏ€* Internal Conversion. , 2016, , .		1