Henrik Koch

List of Publications by Year in Descending Order

155 papers	15,337 citations	49 h-index	123 g-index
168 ext. papers	16,358 ext. citations	3.9 avg, IF	6.34 L-index

#	Paper	IF	Citations
155	Excited state absorption of DNA bases in the gas phase and in chloroform solution: a comparative quantum mechanical study.. *Physical Chemistry Chemical Physics*, **2022**,	3.6	1
154	The effect of midbond functions on interaction energies computed using MP2 and CCSD(T). *Journal of Computational Chemistry*, **2022**, 43, 121-131	3.5	1
153	Molecular orbital theory in cavity QED environments.. *Nature Communications*, **2022**, 13, 1368	17.4	3
152	Linear-Scaling Implementation of Multilevel Hartree-Fock Theory. *Journal of Chemical Theory and Computation*, **2021**,	6.4	2
151	Predictions of Pre-edge Features in Time-Resolved Near-Edge X-ray Absorption Fine Structure Spectroscopy from Hole-Hole Tamm-Dancoff-Approximated Density Functional Theory. *Journal of Chemical Theory and Computation*, **2021**, 17, 7120-7133	6.4	0
150	Intermolecular interactions in optical cavities: An ab initio QED study. *Journal of Chemical Physics*, **2021**, 154, 094113	3.9	31
149	Equation-of-motion coupled-cluster method with double electron-attaching operators: Theory, implementation, and benchmarks. *Journal of Chemical Physics*, **2021**, 154, 114115	3.9	9
148	Describing ground and excited state potential energy surfaces for molecular photoswitches using coupled cluster models. *Journal of Computational Chemistry*, **2021**, 42, 1419-1429	3.5	1
147	New and Efficient Implementation of CC3. *Journal of Chemical Theory and Computation*, **2021**, 17, 117-126	6.4	13
146	Biorthonormal Formalism for Nonadiabatic Coupled Cluster Dynamics. *Journal of Chemical Theory and Computation*, **2021**, 17, 127-138	6.4	0
145	Energy-Based Molecular Orbital Localization in a Specific Spatial Region. *Journal of Chemical Theory and Computation*, **2021**, 17, 139-150	6.4	6
144	Multilevel CC2 and CCSD in Reduced Orbital Spaces: Electronic Excitations in Large Molecular Systems. *Journal of Chemical Theory and Computation*, **2021**, 17, 714-726	6.4	9
143	Multilevel Density Functional Theory. *Journal of Chemical Theory and Computation*, **2021**, 17, 791-803	6.4	8
142	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	6.4	6
141	Strong Coupling between Localized Surface Plasmons and Molecules by Coupled Cluster Theory. *Nano Letters*, **2021**, 21, 6664-6670	11.5	9
140	Transient resonant Auger-Meitner spectra of photoexcited thymine. *Faraday Discussions*, **2021**, 228, 555-570	3.6	2
139	Combining multilevel Hartree-Fock and multilevel coupled cluster approaches with molecular mechanics: a study of electronic excitations in solutions. *Physical Chemistry Chemical Physics*, **2021**, 23, 4413-4425	3.6	8

138	Coupled Cluster Theory for Molecular Polaritons: Changing Ground and Excited States. *Physical Review X*, **2020**, 10,	9.1	34
137	e 1.0: An open source electronic structure program with emphasis on coupled cluster and multilevel methods. *Journal of Chemical Physics*, **2020**, 152, 184103	3.9	34
136	Accurate Description of Photoionization Dynamical Parameters. *Journal of Physical Chemistry Letters*, **2020**, 11, 5330-5337	6.4	13
135	Multilevel CC2 and CCSD Methods with Correlated Natural Transition Orbitals. *Journal of Chemical Theory and Computation*, **2020**, 16, 179-189	6.4	15
134	Accelerated multimodel Newton-type algorithms for faster convergence of ground and excited state coupled cluster equations. *Journal of Chemical Physics*, **2020**, 153, 014104	3.9	4
133	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	6.4	10
132	Time-dependent coupled-cluster theory for ultrafast transient-absorption spectroscopy. *Physical Review A*, **2020**, 102,	2.6	7
131	X-ray and UV Spectra of Glycine within Coupled Cluster Linear Response Theory. *Journal of Physical Chemistry A*, **2019**, 123, 9701-9711	2.8	7
130	An Orbital Invariant Similarity Constrained Coupled Cluster Model. *Journal of Chemical Theory and Computation*, **2019**, 15, 5386-5397	6.4	4
129	An efficient algorithm for Cholesky decomposition of electron repulsion integrals. *Journal of Chemical Physics*, **2019**, 150, 194112	3.9	27
128	Observation of Ultrafast Intersystem Crossing in Thymine by Extreme Ultraviolet Time-Resolved Photoelectron Spectroscopy. *Journal of Physical Chemistry A*, **2019**, 123, 6897-6903	2.8	19
127	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	3.9	6
126	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	1.4	21
125	A theoretical and experimental benchmark study of core-excited states in nitrogen. *Journal of Chemical Physics*, **2018**, 148, 064106	3.9	21
124	Large-Scale Electron Correlation Calculations: Rank-Reduced Full Configuration Interaction. *Journal of Chemical Theory and Computation*, **2018**, 14, 4139-4150	6.4	21
123	Probing ultrafast π/nπ internal conversion in organic chromophores via K-edge resonant absorption. *Nature Communications*, **2017**, 8, 29	17.4	101
122	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	2.8	7
121	Density-Based Multilevel Hartree-Fock Model. *Journal of Chemical Theory and Computation*, **2017**, 13, 5282-5290	6.4	20

120	Resolving the Notorious Case of Conical Intersections for Coupled Cluster Dynamics. *Journal of Physical Chemistry Letters*, **2017**, 8, 4801-4807	6.4	22
119	Tautomerization of Thymine Using Ultraviolet Light. *Langmuir*, **2017**, 33, 9666-9672	4	2
118	Crossing conditions in coupled cluster theory. *Journal of Chemical Physics*, **2017**, 147, 164105	3.9	31
117	Correlated natural transition orbitals for core excitation energies in multilevel coupled cluster models. *Journal of Chemical Physics*, **2017**, 146, 144109	3.9	22
116	A ReaxFF force field for sodium intrusion in graphitic cathodes. *Physical Chemistry Chemical Physics*, **2016**, 18, 31431-31440	3.6	13
115	Chemically accurate energy barriers of small gas molecules moving through hexagonal water rings. *Physical Chemistry Chemical Physics*, **2016**, 18, 17831-5	3.6	2
114	Near-Edge X-ray Absorption Fine Structure within Multilevel Coupled Cluster Theory. *Journal of Chemical Theory and Computation*, **2016**, 12, 2633-43	6.4	29
113	Optical Rotation from Coupled Cluster and Density Functional Theory: The Role of Basis Set Convergence. *Journal of Chemical Theory and Computation*, **2016**, 12, 535-48	6.4	18
112	Transient NEXAFS Spectroscopy at the Oxygen Edge: Pinning Down π/n* Internal Conversion **2016**,		1
111	Potential Energy Surfaces and Charge Transfer of PAH-Sodium-PAH Complexes. *ChemPhysChem*, **2016**, 17, 2908-15	3.2	3
110	The multilevel CC3 coupled cluster model. *Journal of Chemical Physics*, **2016**, 145, 044111	3.9	28
109	Optical Rotation Calculations for a Set of Pyrrole Compounds. *Journal of Physical Chemistry A*, **2016**, 120, 7351-60	2.8	12
108	Optical Rotation Calculations for Fluorinated Alcohols, Amines, Amides, and Esters. *Journal of Physical Chemistry A*, **2016**, 120, 7973-7986	2.8	9
107	Density Functional Theory Study on the Interactions of Metal Ions with Long Chain Deprotonated Carboxylic Acids. *Journal of Physical Chemistry A*, **2015**, 119, 10195-203	2.8	28
106	Communication: X-ray absorption spectra and core-ionization potentials within a core-valence separated coupled cluster framework. *Journal of Chemical Physics*, **2015**, 143, 181103	3.9	110
105	The Dalton quantum chemistry program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 269-284	7.9	956
104	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	3.9	22
103	Multi-level coupled cluster theory. *Journal of Chemical Physics*, **2014**, 141, 224105	3.9	36

102	Assessment of density functionals for van der Waals complexes of sodium and benzene. *Molecular Physics*, **2013**, 111, 1211-1218	1.7	5
101	The extended CC2 model ECC2. *Molecular Physics*, **2013**, 111, 1109-1118	1.7	16
100	The CCSD(T) model with Cholesky decomposition of orbital energy denominators. *International Journal of Quantum Chemistry*, **2011**, 111, 349-355	2.1	8
99	Cholesky Decomposition Techniques in Electronic Structure Theory. *Challenges and Advances in Computational Chemistry and Physics*, **2011**, 301-343	0.7	61
98	Cholesky decomposition-based definition of atomic subsystems in electronic structure calculations. *Journal of Chemical Physics*, **2010**, 132, 204105	3.9	18
97	Coupled cluster response theory in parameter subspaces. *International Journal of Quantum Chemistry*, **2009**, 109, 708-716	2.1	1
96	The benzene-argon ground-state intermolecular potential energy surface revisited. *Journal of Physical Chemistry A*, **2009**, 113, 5212-6	2.8	19
95	Method specific Cholesky decomposition: coulomb and exchange energies. *Journal of Chemical Physics*, **2008**, 129, 134107	3.9	48
94	Variation of polarizability in the [4n+2] annulene series: from [22]- to [66]-annulene. *Physical Chemistry Chemical Physics*, **2008**, 10, 361-5	3.6	14
93	Accurate ab initio density fitting for multiconfigurational self-consistent field methods. *Journal of Chemical Physics*, **2008**, 129, 024113	3.9	145
92	Coupled cluster calculations of interaction energies in benzene–fluorobenzene van der Waals complexes. *Chemical Physics Letters*, **2007**, 441, 332-335	2.5	13
91	Basis set limits of the second order Moller-Plesset correlation energies of water, methane, acetylene, ethylene, and benzene. *Journal of Chemical Physics*, **2007**, 127, 144104	3.9	27
90	Carbon nanorings: A challenge to theoretical chemistry. *ChemPhysChem*, **2006**, 7, 2503-7	3.2	34
89	Fast noniterative orbital localization for large molecules. *Journal of Chemical Physics*, **2006**, 125, 174101	3.9	119
88	Ab initio potential-energy surface and rovibrational states of the HCN-HCl complex. *Journal of Chemical Physics*, **2006**, 124, 204315	3.9	11
87	Ab initio calculation of optical rotation in (P)-(+)-[4]triangulane. *Journal of the American Chemical Society*, **2005**, 127, 1368-9	16.4	72
86	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, 8887-97	3.9	99
85	Polarizabilities of small annulenes from Cholesky CC2 linear response theory. *Chemical Physics Letters*, **2004**, 390, 170-175	2.5	21

84	Origin invariant calculation of optical rotation without recourse to London orbitals. *Chemical Physics Letters*, **2004**, 393, 319-326	2.5	142
83	Argon broadening of the 13CO R(0) and R(7) transitions in the fundamental band at temperatures between 80 and 297 K: comparison between experiment and theory. *Journal of Molecular Spectroscopy*, **2003**, 222, 131-141	1.3	19
82	Coupled cluster calculations of the vertical excitation energies of tetracyanoethylene. *Journal of Chemical Physics*, **2003**, 118, 8216-8222	3.9	12
81	Reduced scaling in electronic structure calculations using Cholesky decompositions. *Journal of Chemical Physics*, **2003**, 118, 9481-9484	3.9	342
80	Study of the benzene?N2 intermolecular potential-energy surface. *Journal of Chemical Physics*, **2003**, 118, 1230-1241	3.9	15
79	Benzene–argon triplet intermolecular potential energy surface. *Journal of Chemical Physics*, **2003**, 119, 4762-4767	3.9	18
78	Computational and experimental investigation of intermolecular states and forces in the benzene–helium van der Waals complex. *Journal of Chemical Physics*, **2003**, 119, 12956-12964	3.9	27
77	Theoretical absorption spectrum of the Ar–CO van der Waals complex. *Journal of Chemical Physics*, **2003**, 118, 9596-9607	3.9	8
76	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	3.9	30
75	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	3.9	57
74	Rovibrational structure of the Ar–CO complex based on a novel three-dimensional ab initio potential. *Journal of Chemical Physics*, **2002**, 117, 6562-6572	3.9	45
73	A coupled cluster calculation of the spectrum of urea. *Chemical Physics Letters*, **2001**, 348, 469-476	2.5	9
72	Comment on "The importance of high-order correlation effects for the CO–CO interaction potential" [Chem. Phys. Lett. 314 (1999) 326]. *Chemical Physics Letters*, **2001**, 334, 419-423	2.5	22
71	Gauge invariant coupled cluster response theory using optimized nonorthogonal orbitals. *Journal of Chemical Physics*, **2001**, 114, 6983-6993	3.9	73
70	The helium–neon– and argon–cyclopropane van der Waals complexes: Ab initio ground state intermolecular potential energy surfaces and intermolecular dynamics. *Journal of Chemical Physics*, **2001**, 115, 8431-8439	3.9	78
69	Propagator Calculations of Electronic Spectra of Photochromic Spirooxazines. *Molecular Crystals and Liquid Crystals*, **2000**, 345, 89-94		1
68	Size-intensive decomposition of orbital energy denominators. *Journal of Chemical Physics*, **2000**, 113, 508-513	3.9	41
67	Atomic integral driven second order polarization propagator calculations of the excitation spectra of naphthalene and anthracene. *Journal of Chemical Physics*, **2000**, 112, 4173-4185	3.9	122

66	Theoretical electronic absorption and natural circular dichroism spectra of (l)-trans-cyclooctene. *Journal of Chemical Physics*, **2000**, 112, 2139-2147	3.9	25
65	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	3.9	21
64	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	3.9	74
63	Gauge invariant coupled cluster response theory. *Journal of Chemical Physics*, **1999**, 110, 8318-8327	3.9	87
62	Coupled cluster response calculation of natural chiroptical spectra. *Journal of Chemical Physics*, **1999**, 110, 2883-2892	3.9	72
61	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	3.9	44
60	Ab initio calculation of the frequency-dependent interaction induced hyperpolarizability of Ar2. *Journal of Chemical Physics*, **1999**, 110, 2872-2882	3.9	46
59	Accurate intermolecular ground state potential of the Ar–N2 complex. *Journal of Chemical Physics*, **1999**, 110, 8525-8532	3.9	34
58	Ground state benzene–argon intermolecular potential energy surface. *Journal of Chemical Physics*, **1999**, 111, 198-204	3.9	86
57	Benzene-argon S1 intermolecular potential energy surface. *Journal of Chemical Physics*, **1999**, 111, 5922-5928	3.9	43
56	A second-order doubles correction to excitation energies in the random-phase approximation. *Chemical Physics Letters*, **1998**, 284, 47-55	2.5	36
55	The Hartree–Fock magnetizability of C60. *Chemical Physics Letters*, **1998**, 285, 205-209	2.5	15
54	Basis-set convergence in correlated calculations on Ne, N2, and H2O. *Chemical Physics Letters*, **1998**, 286, 243-252	2.5	1786
53	Gauge invariance of the coupled cluster oscillator strength. *Chemical Physics Letters*, **1998**, 293, 251-260	2.5	29
52	The vibrational and temperature dependence of the indirect nuclear spin–spin coupling constants of the oxonium (H3O+) and hydroxyl (OH−) ions. *Chemical Physics*, **1998**, 238, 385-399	2.3	46
51	Accurate ab initio rovibronic spectrum of the X 1Σg+ and B 1Δu+ states in Ar2. *Journal of Chemical Physics*, **1998**, 109, 10255-10262	3.9	31
50	On the time-dependent Lagrangian approach in quantum chemistry. *Journal of Chemical Physics*, **1998**, 108, 5194-5204	3.9	19
49	Integral-direct coupled cluster calculations of frequency-dependent polarizabilities, transition probabilities and excited-state properties. *Journal of Chemical Physics*, **1998**, 108, 2801-2816	3.9	178

48	The Cotton–Mouton effect of liquid water. Part II: The semi-continuum model. *Journal of Chemical Physics*, **1998**, 108, 599-603	3.9	18
47	The benzene–argon complex: A ground and excited state ab initio study. *Journal of Chemical Physics*, **1998**, 108, 2784-2790	3.9	139
46	C24: Ring or fullerene?. *Journal of Chemical Physics*, **1998**, 108, 3213-3217	3.9	26
45	Comment on "Frequency-dependent equation-of-motion coupled cluster hyperpolarizabilities: Resolution of the discrepancy between theory and experiment for HF?" [J. Chem. Phys. 107, 10823 (1997)]. *Journal of Chemical Physics*, **1998**, 109, 3293-3295	3.9	11
44	Comment on "Response to "Comment on 'Frequency-dependent equation-of-motion coupled cluster hyperpolarizabilities: Resolution of the discrepancy between theory and experiment for HF?'" [J. Chem. Phys. 109, 9201 (1998)]. *Journal of Chemical Physics*, **1998**, 109, 9204-9204	3.9	2
43	The CC3 model: An iterative coupled cluster approach including connected triples. *Journal of Chemical Physics*, **1997**, 106, 1808-1818	3.9	362
42	First-order one-electron properties in the integral-direct coupled cluster singles and doubles model. *Journal of Chemical Physics*, **1997**, 107, 849-866	3.9	117
41	Basis-set convergence of correlated calculations on water. *Journal of Chemical Physics*, **1997**, 106, 9639-9646	3.9	1932
40	Coupled cluster response functions revisited. *Journal of Chemical Physics*, **1997**, 106, 8059-8072	3.9	97
39	A systematic ab initio study of the water dimer in hierarchies of basis sets and correlation models. *Theoretical Chemistry Accounts*, **1997**, 97, 150-157	1.9	173
38	Multiple basis sets in calculations of triples corrections in coupled-cluster theory. *Theoretical Chemistry Accounts*, **1997**, 97, 164-176	1.9	79
37	Frequency-dependent first hyperpolarizabilities using coupled cluster quadratic response theory. *Chemical Physics Letters*, **1997**, 269, 428-434	2.5	119
36	Full configuration–interaction and state of the art correlation calculations on water in a valence double-zeta basis with polarization functions. *Journal of Chemical Physics*, **1996**, 104, 8007-8015	3.9	235
35	Surprising cases of divergent behavior in Mo/ller–Plesset perturbation theory. *Journal of Chemical Physics*, **1996**, 105, 5082-5090	3.9	175
34	Large-scale calculations of excitation energies in coupled cluster theory: The singlet excited states of benzene. *Journal of Chemical Physics*, **1996**, 105, 6921-6939	3.9	173
33	Efficient parallel implementation of response theory: Calculations of the second hyperpolarizability of polyacenes. *Chemical Physics Letters*, **1996**, 253, 1-7	2.5	45
32	Dynamic CCSD polarisabilities of CHF3 and CHCl3. *Chemical Physics Letters*, **1996**, 253, 373-376	2.5	11
31	Excitation energies of H2O, N2 and C2 in full configuration interaction and coupled cluster theory. *Chemical Physics Letters*, **1996**, 256, 185-194	2.5	210

30	On the inherent divergence in the Møller-Plesset series. The neon atom as a test case. *Chemical Physics Letters*, **1996**, 261, 369-378	2.5	74
29	Integral direct calculation of CC2 excitation energies: singlet excited states of benzene. *Chemical Physics Letters*, **1996**, 263, 530-539	2.5	51
28	Perturbative triple excitation corrections to coupled cluster singles and doubles excitation energies. *Journal of Chemical Physics*, **1996**, 105, 1451-1459	3.9	196
27	The molecular structure of ferrocene. *Journal of Chemical Physics*, **1996**, 104, 9528-9530	3.9	92
26	The integral-direct coupled cluster singles and doubles model. *Journal of Chemical Physics*, **1996**, 104, 4157-4165	3.9	146
25	Random-phase calculations of frequency-dependent polarizabilities and hyperpolarizabilities of long polyene chains. *Physical Review B*, **1995**, 51, 14949-14957	3.3	29
24	SCF calculations of the NMR shielding tensor for the ethylenic carbon atom in C3Cl4. *Molecular Physics*, **1995**, 85, 671-673	1.7	5
23	Response functions in the CC3 iterative triple excitation model. *Journal of Chemical Physics*, **1995**, 103, 7429-7441	3.9	451
22	The second-order approximate coupled cluster singles and doubles model CC2. *Chemical Physics Letters*, **1995**, 243, 409-418	2.5	1409
21	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	2.5	217
20	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	3.9	18
19	Calculation of size-intensive transition moments from the coupled cluster singles and doubles linear response function. *Journal of Chemical Physics*, **1994**, 100, 4393-4400	3.9	192
18	Brueckner coupled cluster response functions. *International Journal of Quantum Chemistry*, **1994**, 49, 835-848	2.1	20
17	Calculation of frequency-dependent polarizabilities using coupled-cluster response theory. *Chemical Physics Letters*, **1994**, 219, 30-35	2.5	106
16	A direct atomic orbital driven implementation of the coupled cluster singles and doubles (CCSD) model. *Chemical Physics Letters*, **1994**, 228, 233-238	2.5	115
15	Frequency dependent hyperpolarizabilities of polyynes. *Journal of Chemical Physics*, **1993**, 98, 7229-7235	3.9	31
14	Direct atomic orbital based self-consistent-field calculations of nonlinear molecular properties. Application to the frequency dependent hyperpolarizability of para-nitroaniline. *Journal of Chemical Physics*, **1993**, 98, 6417-6423	3.9	87
13	Comparison of coupled-cluster and Brueckner coupled-cluster calculations of molecular properties. *Chemical Physics Letters*, **1993**, 211, 94-100	2.5	64

12	Linear superposition of optimized non-orthogonal Slater determinants for singlet states. *Chemical Physics Letters*, **1993**, 212, 193-200	2.5	20
11	Quartic coupled cluster force fields for the diazene isomers. *Chemical Physics Letters*, **1993**, 215, 576-581	2.5	8
10	Large scale random phase calculations for direct self-consistent field wavefunctions. *Chemical Physics*, **1993**, 172, 13-20	2.3	28
9	A variational matrix decomposition applied to full configuration-interaction calculations. *Chemical Physics Letters*, **1992**, 198, 51-58	2.5	6
8	Analytical calculation of full configuration interaction response properties: Application to Be. *Journal of Chemical Physics*, **1991**, 95, 7479-7485	3.9	50
7	Branching ratios for the dissociative decay of triplet H2. *Physical Review A*, **1991**, 44, 4171-4179	2.6	29
6	Coupled cluster response functions. *Journal of Chemical Physics*, **1990**, 93, 3333-3344	3.9	885
5	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	3.9	491
4	Determination of the transition dipole moment □þ(R) in H2 from the measurement of vibrational wave functions. *Journal of Chemical Physics*, **1990**, 93, 3887-3890	3.9	6
3	Coupled cluster energy derivatives. Analytic Hessian for the closed-shell coupled cluster singles and doubles wave function: Theory and applications. *Journal of Chemical Physics*, **1990**, 92, 4924-4940	3.9	214
2	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	2.5	13
1	Direct iterative RPA calculations. Applications to ethylene, benzene and cytosine. *Chemical Physics*, **1988**, 119, 297-306	2.3	36