Henrik Koch

List of Publications by Citations

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	Basis-set convergence of correlated calculations on water. *Journal of Chemical Physics*, **1997**, 106, 9639-9646	3.9	1932
154	Basis-set convergence in correlated calculations on Ne, N2, and H2O. *Chemical Physics Letters*, **1998**, 286, 243-252	2.5	1786
153	The second-order approximate coupled cluster singles and doubles model CC2. *Chemical Physics Letters*, **1995**, 243, 409-418	2.5	1409
152	The Dalton quantum chemistry program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 269-284	7.9	956
151	Coupled cluster response functions. *Journal of Chemical Physics*, **1990**, 93, 3333-3344	3.9	885
150	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
149	Response functions in the CC3 iterative triple excitation model. *Journal of Chemical Physics*, **1995**, 103, 7429-7441	3.9	451
148	The CC3 model: An iterative coupled cluster approach including connected triples. *Journal of Chemical Physics*, **1997**, 106, 1808-1818	3.9	362
147	Reduced scaling in electronic structure calculations using Cholesky decompositions. *Journal of Chemical Physics*, **2003**, 118, 9481-9484	3.9	342
146	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
145	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
144	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
143	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
142	Perturbative triple excitation corrections to coupled cluster singles and doubles excitation energies. *Journal of Chemical Physics*, **1996**, 105, 1451-1459	3.9	196
141	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
140	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
139	Surprising cases of divergent behavior in Mo/ller Plesset perturbation theory. *Journal of Chemical Physics*, **1996**, 105, 5082-5090	3.9	175

138	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
137	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
136	The integral-direct coupled cluster singles and doubles model. *Journal of Chemical Physics*, **1996**, 104, 4157-4165	3.9	146
135	Accurate ab initio density fitting for multiconfigurational self-consistent field methods. *Journal of Chemical Physics*, **2008**, 129, 024113	3.9	145
134	Origin invariant calculation of optical rotation without recourse to London orbitals. *Chemical Physics Letters*, **2004**, 393, 319-326	2.5	142
133	The benzene□rgon complex: A ground and excited state ab initio study. *Journal of Chemical Physics* , **1998**, 108, 2784-2790	3.9	139
132	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
131	Frequency-dependent first hyperpolarizabilities using coupled cluster quadratic response theory. *Chemical Physics Letters*, **1997**, 269, 428-434	2.5	119
130	Fast noniterative orbital localization for large molecules. *Journal of Chemical Physics*, **2006**, 125, 174101	3.9	119
129	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
128	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
127	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
126	Calculation of frequency-dependent polarizabilities using coupled-cluster response theory. *Chemical Physics Letters*, **1994**, 219, 30-35	2.5	106
125	Probing ultrafast □/n□ internal conversion in organic chromophores via K-edge resonant absorption. *Nature Communications*, **2017**, 8, 29	17.4	101
124	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
123	Coupled cluster response functions revisited. *Journal of Chemical Physics*, **1997**, 106, 8059-8072	3.9	97
122	The molecular structure of ferrocene. *Journal of Chemical Physics*, **1996**, 104, 9528-9530	3.9	92
121	Gauge invariant coupled cluster response theory. *Journal of Chemical Physics*, **1999**, 110, 8318-8327	3.9	87

120	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
119	Ground state benzene–argon intermolecular potential energy surface. *Journal of Chemical Physics*, **1999**, 111, 198-204	3.9	86
118	Multiple basis sets in calculations of triples corrections in coupled-cluster theory. *Theoretical Chemistry Accounts*, **1997**, 97, 164-176	1.9	79
117	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
116	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
115	On the inherent divergence in the M–ller-Plesset series. The neon atom – a test case. *Chemical Physics Letters*, **1996**, 261, 369-378	2.5	74
114	Gauge invariant coupled cluster response theory using optimized nonorthogonal orbitals. *Journal of Chemical Physics*, **2001**, 114, 6983-6993	3.9	73
113	Ab initio calculation of optical rotation in (P)-(+)-[4]triangulane. *Journal of the American Chemical Society*, **2005**, 127, 1368-9	16.4	72
112	Coupled cluster response calculation of natural chiroptical spectra. *Journal of Chemical Physics*, **1999**, 110, 2883-2892	3.9	72
111	Comparison of coupled-cluster and Brueckner coupled-cluster calculations of molecular properties. *Chemical Physics Letters*, **1993**, 211, 94-100	2.5	64
110	Cholesky Decomposition Techniques in Electronic Structure Theory. *Challenges and Advances in Computational Chemistry and Physics*, **2011**, 301-343	0.7	61
109	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
108	Integral direct calculation of CC2 excitation energies: singlet excited states of benzene. *Chemical Physics Letters*, **1996**, 263, 530-539	2.5	51
107	Analytical calculation of full configuration interaction response properties: Application to Be. *Journal of Chemical Physics*, **1991**, 95, 7479-7485	3.9	50
106	Method specific Cholesky decomposition: coulomb and exchange energies. *Journal of Chemical Physics*, **2008**, 129, 134107	3.9	48
105	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
104	Ab initio calculation of the frequency-dependent interaction induced hyperpolarizability of Ar2. *Journal of Chemical Physics*, **1999**, 110, 2872-2882	3.9	46
103	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

102	Efficient parallel implementation of response theory: Calculations of the second hyperpolarizability of polyacenes. *Chemical Physics Letters*, **1996**, 253, 1-7	2.5	45
101	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
100	Benzene-argon S1 intermolecular potential energy surface. *Journal of Chemical Physics*, **1999**, 111, 5922-5928	3.9	43
99	Size-intensive decomposition of orbital energy denominators. *Journal of Chemical Physics*, **2000**, 113, 508-513	3.9	41
98	Multi-level coupled cluster theory. *Journal of Chemical Physics*, **2014**, 141, 224105	3.9	36
97	A second-order doubles correction to excitation energies in the random-phase approximation. *Chemical Physics Letters*, **1998**, 284, 47-55	2.5	36
96	Direct iterative RPA calculations. Applications to ethylene, benzene and cytosine. *Chemical Physics*, **1988**, 119, 297-306	2.3	36
95	Coupled Cluster Theory for Molecular Polaritons: Changing Ground and Excited States. *Physical Review X*, **2020**, 10,	9.1	34
94	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
93	Carbon nanorings: A challenge to theoretical chemistry. *ChemPhysChem*, **2006**, 7, 2503-7	3.2	34
92	Accurate intermolecular ground state potential of the Ar□2 complex. *Journal of Chemical Physics*, **1999**, 110, 8525-8532	3.9	34
91	Crossing conditions in coupled cluster theory. *Journal of Chemical Physics*, **2017**, 147, 164105	3.9	31
90	Accurate ab initio rovibronic spectrum of the X 1□g+ and B 1□u+ states in Ar2. *Journal of Chemical Physics*, **1998**, 109, 10255-10262	3.9	31
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88	Intermolecular interactions in optical cavities: An ab initio QED study. *Journal of Chemical Physics*, **2021**, 154, 094113	3.9	31
87	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
86	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
85	Gauge invariance of the coupled cluster oscillator strength. *Chemical Physics Letters*, **1998**, 293, 251-260	2.5	29

84	Random-phase calculations of frequency-dependent polarizabilities and hyperpolarizabilities of long polyene chains. *Physical Review B*, **1995**, 51, 14949-14957	3.3	29
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82	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
81	Large scale random phase calculations for direct self-consistent field wavefunctions. *Chemical Physics*, **1993**, 172, 13-20	2.3	28
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79	An efficient algorithm for Cholesky decomposition of electron repulsion integrals. *Journal of Chemical Physics*, **2019**, 150, 194112	3.9	27
78	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
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75	Theoretical electronic absorption and natural circular dichroism spectra of (+)-trans-cyclooctene. *Journal of Chemical Physics*, **2000**, 112, 2139-2147	3.9	25
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73	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
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69	Large-Scale Electron Correlation Calculations: Rank-Reduced Full Configuration Interaction. *Journal of Chemical Theory and Computation*, **2018**, 14, 4139-4150	6.4	21
68	Polarizabilities of small annulenes from Cholesky CC2 linear response theory. *Chemical Physics Letters*, **2004**, 390, 170-175	2.5	21
67	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

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64	Brueckner coupled cluster response functions. *International Journal of Quantum Chemistry*, **1994**, 49, 835-848	2.1	20
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61	The benzene-argon ground-state intermolecular potential energy surface revisited. *Journal of Physical Chemistry A*, **2009**, 113, 5212-6	2.8	19
60	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
59	On the time-dependent Lagrangian approach in quantum chemistry. *Journal of Chemical Physics*, **1998**, 108, 5194-5204	3.9	19
58	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
57	Cholesky decomposition-based definition of atomic subsystems in electronic structure calculations. *Journal of Chemical Physics*, **2010**, 132, 204105	3.9	18
56	Benzene□rgon triplet intermolecular potential energy surface. *Journal of Chemical Physics*, **2003**, 119, 4762-4767	3.9	18
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50	Multilevel CC2 and CCSD Methods with Correlated Natural Transition Orbitals. *Journal of Chemical Theory and Computation*, **2020**, 16, 179-189	6.4	15
49	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

48	Accurate Description of Photoionization Dynamical Parameters. *Journal of Physical Chemistry Letters*, **2020**, 11, 5330-5337	6.4	13
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46	Coupled cluster calculations of interaction energies in benzene–fluorobenzene van der Waals complexes. *Chemical Physics Letters*, **2007**, 441, 332-335	2.5	13
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44	New and Efficient Implementation of CC3. *Journal of Chemical Theory and Computation*, **2021**, 17, 117-126	6.4	13
43	Coupled cluster calculations of the vertical excitation energies of tetracyanoethylene. *Journal of Chemical Physics*, **2003**, 118, 8216-8222	3.9	12
42	Optical Rotation Calculations for a Set of Pyrrole Compounds. *Journal of Physical Chemistry A*, **2016**, 120, 7351-60	2.8	12
41	Ab initio potential-energy surface and rovibrational states of the HCN-HCl complex. *Journal of Chemical Physics*, **2006**, 124, 204315	3.9	11
40	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
39	Dynamic CCSD polarisabilities of CHF3 and CHCl3. *Chemical Physics Letters*, **1996**, 253, 373-376	2.5	11
38	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
37	A coupled cluster calculation of the spectrum of urea. *Chemical Physics Letters*, **2001**, 348, 469-476	2.5	9
36	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
35	Optical Rotation Calculations for Fluorinated Alcohols, Amines, Amides, and Esters. *Journal of Physical Chemistry A*, **2016**, 120, 7973-7986	2.8	9
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33	Strong Coupling between Localized Surface Plasmons and Molecules by Coupled Cluster Theory. *Nano Letters*, **2021**, 21, 6664-6670	11.5	9
32	The CCSD(T) model with Cholesky decomposition of orbital energy denominators. *International Journal of Quantum Chemistry*, **2011**, 111, 349-355	2.1	8
31	Theoretical absorption spectrum of the Ar–CO van der Waals complex. *Journal of Chemical Physics*, **2003**, 118, 9596-9607	3.9	8

30	Quartic coupled cluster force fields for the diazene isomers. *Chemical Physics Letters*, **1993**, 215, 576-581	2.5	8
29	Multilevel Density Functional Theory. *Journal of Chemical Theory and Computation*, **2021**, 17, 791-803	6.4	8
28	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
27	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
26	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
25	Time-dependent coupled-cluster theory for ultrafast transient-absorption spectroscopy. *Physical Review A*, **2020**, 102,	2.6	7
24	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
23	A variational matrix decomposition applied to full configuration-interaction calculations. *Chemical Physics Letters*, **1992**, 198, 51-58	2.5	6
22	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
21	Energy-Based Molecular Orbital Localization in a Specific Spatial Region. *Journal of Chemical Theory and Computation*, **2021**, 17, 139-150	6.4	6
20	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
19	Assessment of density functionals for van der Waals complexes of sodium and benzene. *Molecular Physics*, **2013**, 111, 1211-1218	1.7	5
18	SCF calculations of the NMR shielding tensor for the ethylenic carbon atom in C3Cl4. *Molecular Physics*, **1995**, 85, 671-673	1.7	5
17	An Orbital Invariant Similarity Constrained Coupled Cluster Model. *Journal of Chemical Theory and Computation*, **2019**, 15, 5386-5397	6.4	4
16	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
15	Potential Energy Surfaces and Charge Transfer of PAH-Sodium-PAH Complexes. *ChemPhysChem*, **2016**, 17, 2908-15	3.2	3
14	Molecular orbital theory in cavity QED environments.. *Nature Communications*, **2022**, 13, 1368	17.4	3
13	Chemically accurate energy barriers of small gas molecules moving through hexagonal water rings. *Physical Chemistry Chemical Physics*, **2016**, 18, 17831-5	3.6	2

12	Tautomerization of Thymine Using Ultraviolet Light. *Langmuir*, **2017**, 33, 9666-9672	4	2
11	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
10	Linear-Scaling Implementation of Multilevel Hartree-Fock Theory. *Journal of Chemical Theory and Computation*, **2021**,	6.4	2
9	Transient resonant Auger-Meitner spectra of photoexcited thymine. *Faraday Discussions*, **2021**, 228, 555-570	3.6	2
8	Coupled cluster response theory in parameter subspaces. *International Journal of Quantum Chemistry*, **2009**, 109, 708-716	2.1	1
7	Propagator Calculations of Electronic Spectra of Photochromic Spirooxazines. *Molecular Crystals and Liquid Crystals*, **2000**, 345, 89-94		1
6	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
5	Transient NEXAFS Spectroscopy at the Oxygen Edge: Pinning Down π/n Internal Conversion **2016**,		1
4	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
3	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
2	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
1	Biorthonormal Formalism for Nonadiabatic Coupled Cluster Dynamics. *Journal of Chemical Theory and Computation*, **2021**, 17, 127-138	6.4	0