

# Christof Hattig

## List of Publications by Year in descending order

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188  
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17,855  
citations

22099

59  
h-index

13338

130  
g-index

200  
all docs

200  
docs citations

200  
times ranked

9529  
citing authors

#	ARTICLE	IF	CITATIONS
1	Efficient use of the correlation consistent basis sets in resolution of the identity MP2 calculations. <i>Journal of Chemical Physics</i> , 2002, 116, 3175-3183.	1.2	1,671
2	CC2 excitation energy calculations on large molecules using the resolution of the identity approximation. <i>Journal of Chemical Physics</i> , 2000, 113, 5154.	1.2	1,319
3	The Dalton quantum chemistry program system. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2014, 4, 269-284.	6.2	1,166
4	Turbomole. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2014, 4, 91-100.	6.2	867
5	Optimization of auxiliary basis sets for RI-MP2 and RI-CC2 calculations: Core-valence and quintuple- $\zeta$ basis sets for H to Ar and QZVPP basis sets for Li to Kr. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 59-66.	1.3	631
6	TURBOMOLE: Modular program suite for <i>ab initio</i> quantum-chemical and condensed-matter simulations. <i>Journal of Chemical Physics</i> , 2020, 152, 184107.	1.2	616
7	Optimized accurate auxiliary basis sets for RI-MP2 and RI-CC2 calculations for the atoms Rb to Rn. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 587-597.	0.5	577
8	Response functions from Fourier component variational perturbation theory applied to a time-averaged quasienergy. <i>International Journal of Quantum Chemistry</i> , 1998, 68, 1-52.	1.0	497
9	Explicitly Correlated Electrons in Molecules. <i>Chemical Reviews</i> , 2012, 112, 4-74.	23.0	487
10	Geometry optimizations with the coupled-cluster model CC2 using the resolution-of-the-identity approximation. <i>Journal of Chemical Physics</i> , 2003, 118, 7751-7761.	1.2	443
11	Transition moments and excited-state first-order properties in the coupled-cluster model CC2 using the resolution-of-the-identity approximation. <i>Journal of Chemical Physics</i> , 2002, 117, 6939-6951.	1.2	402
12	Structure Optimizations for Excited States with Correlated Second-Order Methods: CC2 and ADC(2). <i>Advances in Quantum Chemistry</i> , 2005, 50, 37-60.	0.4	386
13	Analytic gradients for excited states in the coupled-cluster model CC2 employing the resolution-of-the-identity approximation. <i>Journal of Chemical Physics</i> , 2003, 119, 5021-5036.	1.2	372
14	Tautomeric selectivity of the excited-state lifetime of guanine/cytosine base pairs: The role of electron-driven proton-transfer processes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 17903-17906.	3.3	290
15	Benchmarking the performance of spin-component scaled CC2 in ground and electronically excited states. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 4119.	1.3	276
16	Communications: Accurate and efficient approximations to explicitly correlated coupled-cluster singles and doubles, CCSD-F12. <i>Journal of Chemical Physics</i> , 2010, 132, 231102.	1.2	259
17	Quintuple- $\zeta$ quality coupled-cluster correlation energies with triple- $\zeta$ basis sets. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 1921-1930.	1.3	244
18	Distributed memory parallel implementation of energies and gradients for second-order Møller-Plesset perturbation theory with the resolution-of-the-identity approximation. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 1159.	1.3	223

#	ARTICLE	IF	CITATIONS
19	Ab Initio Calculation of the Vibrational and Electronic Spectra of trans- and cis-Azobenzene. Journal of the American Chemical Society, 2003, 125, 9821-9827.	6.6	194
20	Excited-State Intramolecular Proton Transfer: A Survey of TDDFT and RI-CC2 Excited-State Potential Energy Surfaces. Journal of Physical Chemistry A, 2005, 109, 3201-3208.	1.1	175
21	Benchmarks for $\sigma \rightarrow \sigma^*$ transitions of aromatic organic molecules: DFT/B3LYP, ADC(2), CC2, SOS-CC2 and SCS-CC2 compared to high-resolution gas-phase data. Physical Chemistry Chemical Physics, 2013, 15, 6623-6630.	1.3	173
22	Coupled-cluster theory with simplified linear-r12 corrections: The CCSD(R12) model. Journal of Chemical Physics, 2005, 122, 084107.	1.2	167
23	Distributed polarizabilities using the topological theory of atoms in molecules. Chemical Physics Letters, 1994, 219, 267-273.	1.2	142
24	Benchmarking two-photon absorption with CC3 quadratic response theory, and comparison with density-functional response theory. Journal of Chemical Physics, 2006, 124, 054322.	1.2	137
25	Polarizabilities of CO, N <sub>2</sub> , HF, Ne, BH, and CH <sup>+</sup> from ab initio calculations: Systematic studies of electron correlation, basis set errors, and vibrational contributions. Journal of Chemical Physics, 1998, 109, 4745-4757.	1.2	127
26	Frequency-dependent first hyperpolarizabilities using coupled cluster quadratic response theory. Chemical Physics Letters, 1997, 269, 428-434.	1.2	125
27	The accuracy of ab initio molecular geometries for systems containing second-row atoms. Journal of Chemical Physics, 2005, 123, 184107.	1.2	125
28	Implementation of RI-CC2 triplet excitation energies with an application to trans-azobenzene. Physical Chemistry Chemical Physics, 2002, 4, 2111-2118.	1.3	122
29	A diagonal orbital-invariant explicitly-correlated coupled-cluster method. Chemical Physics Letters, 2008, 452, 326-332.	1.2	118
30	On the Nature of the Low-Lying Singlet States of 4-(Dimethyl-amino)benzonitrile. Journal of the American Chemical Society, 2004, 126, 7399-7410.	6.6	113
31	Frequency-dependent second hyperpolarizabilities using coupled cluster cubic response theory. Chemical Physics Letters, 1998, 282, 139-146.	1.2	108
32	Quantum-Chemical Investigation of the Structures and Electronic Spectra of the Nucleic Acid Bases at the Coupled Cluster CC2 Level. Journal of Physical Chemistry A, 2007, 111, 5482-5491.	1.1	108
33	Photophysics of Organic Photostabilizers. Ab Initio Study of the Excited-State Deactivation Mechanisms of 2-(2-Hydroxyphenyl)benzotriazole. Journal of Physical Chemistry A, 2006, 110, 6301-6306.	1.1	107
34	A pair natural orbital implementation of the coupled cluster model CC2 for excitation energies. Journal of Chemical Physics, 2013, 139, 084114.	1.2	104
35	The MP2+ $\epsilon$ 12 method in the TURBOMOLE program package. Journal of Computational Chemistry, 2011, 32, 2492-2513.	1.5	98
36	Gauge invariant coupled cluster response theory. Journal of Chemical Physics, 1999, 110, 8318-8327.	1.2	96

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37	Coupled cluster calculations of the optical rotation of S-propylene oxide in gas phase and solution. <i>Chemical Physics Letters</i> , 2005, 401, 385-392.	1.2	94
38	Explicitly correlated PNO-MP2 and PNO-CCSD and their application to the S66 set and large molecular systems. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 22167-22178.	1.3	92
39	Scaled opposite-spin CC2 for ground and excited states with fourth order scaling computational costs. <i>Journal of Chemical Physics</i> , 2011, 134, 184101.	1.2	91
40	Multiphoton transition moments and absorption cross sections in coupled cluster response theory employing variational transition moment functionals. <i>Journal of Chemical Physics</i> , 1998, 108, 8331-8354.	1.2	90
41	Polarizabilities and first hyperpolarizabilities of HF, Ne, and BH from full configuration interaction and coupled cluster calculations. <i>Journal of Chemical Physics</i> , 1999, 111, 1917-1925.	1.2	89
42	Local explicitly correlated second-order Møller-Plesset perturbation theory with pair natural orbitals. <i>Journal of Chemical Physics</i> , 2011, 135, 074107.	1.2	87
43	Local pair natural orbitals for excited states. <i>Journal of Chemical Physics</i> , 2011, 135, 214106.	1.2	87
44	Local explicitly correlated second- and third-order Møller-Plesset perturbation theory with pair natural orbitals. <i>Journal of Chemical Physics</i> , 2012, 136, 204105.	1.2	85
45	Calculation of two-photon absorption strengths with the approximate coupled cluster singles and doubles model CC2 using the resolution-of-identity approximation. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 1175-1184.	1.3	76
46	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 He <sub>2</sub> and Ar <sub>2</sub> . <i>Journal of Chemical Physics</i> , 1999, 111, 10099-10107.	1.2	75
47	Correlated frequency-dependent electronic first hyperpolarizability of small push-pull conjugated chains. <i>Chemical Physics Letters</i> , 2000, 319, 327-334.	1.2	75
48	PERI-CC2: A Polarizable Embedded RI-CC2 Method. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3274-3283.	2.3	75
49	The charge-transfer states in a stacked nucleobase dimer complex: A benchmark study. <i>Journal of Computational Chemistry</i> , 2011, 32, 1217-1227.	1.5	73
50	Perturbative triples correction for local pair natural orbital based explicitly correlated CCSD(F12*) using Laplace transformation techniques. <i>Journal of Chemical Physics</i> , 2016, 145, 234107.	1.2	72
51	Inclusion of the (T) triples correction into the linear-r12 corrected coupled-cluster model CCSD(R12). <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2306-2317.	1.0	69
52	Ab initio study of the individual interaction energy components in the ground state of the mercury dimer. <i>Molecular Physics</i> , 1996, 89, 139-156.	0.8	66
53	Coupled cluster calculations of the ground state potential and interaction induced electric properties of the mixed dimers of helium, neon and argon. <i>Molecular Physics</i> , 2004, 102, 101-110.	0.8	65
54	Formic Acid-Assisted Selective Hydrogenolysis of 5-Hydroxymethylfurfural to 2,5-Dimethylfuran over Bifunctional Pd Nanoparticles Supported on N-Doped Mesoporous Carbon. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 6807-6815.	7.2	65

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55	Gauge-origin independent magneto-optical activity within coupled cluster response theory. <i>Journal of Chemical Physics</i> , 2000, 113, 3561-3572.	1.2	64
56	Accurate computational thermochemistry from explicitly correlated coupled-cluster theory. <i>Theoretical Chemistry Accounts</i> , 2010, 126, 289-304.	0.5	64
57	Correlated frequency-dependent polarizabilities and dispersion coefficients in the time-dependent second-order Møller-Plesset approximation. <i>Chemical Physics Letters</i> , 1995, 233, 359-370.	1.2	60
58	TDMP2 Calculation of Dynamic Multipole Polarizabilities and Dispersion Coefficients of the Noble Gases Ar, Kr, Xe, and Rn. <i>The Journal of Physical Chemistry</i> , 1996, 100, 6243-6248.	2.9	60
59	First-order properties for triplet excited states in the approximated coupled cluster model CC2 using an explicitly spin coupled basis. <i>Journal of Chemical Physics</i> , 2002, 116, 5401-5410.	1.2	60
60	The effect of intermolecular interactions on the electric properties of helium and argon. III. Quantum statistical calculations of the dielectric second virial coefficients. <i>Journal of Chemical Physics</i> , 2002, 117, 2609-2618.	1.2	60
61	A scaling PNO-MP2 method using a hybrid OSV-PNO approach with an iterative direct generation of OSVs. <i>Molecular Physics</i> , 2013, 111, 2463-2476.	0.8	60
62	TDMP2 calculation of dynamic multipole polarizabilities and dispersion coefficients for the halogen anions F <sup>-</sup> , Cl <sup>-</sup> , Br <sup>-</sup> and I <sup>-</sup> . <i>Journal of Chemical Physics</i> , 1998, 108, 3863-3870.	1.2	59
63	A Lagrangian, integral-density direct formulation and implementation of the analytic CCSD and CCSD(T) gradients. <i>Journal of Chemical Physics</i> , 2003, 118, 2985-2998.	1.2	57
64	Calculation of frequency-dependent polarizabilities using the approximate coupled-cluster triples model CC3. <i>Journal of Chemical Physics</i> , 2003, 118, 1292-1300.	1.2	56
65	Distributed first and second order hyperpolarizabilities: An improved calculation of nonlinear optical susceptibilities of molecular crystals. <i>Journal of Chemical Physics</i> , 2000, 112, 6161-6172.	1.2	55
66	Intramolecular Charge-Transfer Mechanism in Quinolidines: The Role of the Amino Twist Angle. <i>Journal of the American Chemical Society</i> , 2006, 128, 15672-15682.	6.6	54
67	Auxiliary basis sets for density-fitted correlated wavefunction calculations: weighted core-valence and ECP basis sets for post-d elements. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 6549.	1.3	53
68	Cauchy moments and dispersion coefficients using coupled cluster linear response theory. <i>Journal of Chemical Physics</i> , 1997, 107, 10592-10598.	1.2	51
69	A pair natural orbital based implementation of ADC(2)-x: Perspectives and challenges for response methods for singly and doubly excited states in large molecules. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 35-44.	1.1	51
70	The effect of intermolecular interactions on the electric properties of helium and argon. II. The dielectric, refractivity, Kerr, and hyperpolarizability second virial coefficients. <i>Journal of Chemical Physics</i> , 1999, 111, 10108-10118.	1.2	48
71	Coupled-cluster response theory with linear-r12 corrections: The CC2-R12 model for excitation energies. <i>Journal of Chemical Physics</i> , 2006, 124, 044112.	1.2	48
72	A pair natural orbital based implementation of CCSD excitation energies within the framework of linear response theory. <i>Journal of Chemical Physics</i> , 2018, 148, 134102.	1.2	48

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73	Ab initio calculation of the frequency-dependent interaction induced hyperpolarizability of Ar <sub>2</sub> . Journal of Chemical Physics, 1999, 110, 2872-2882.	1.2	46
74	High-order correlation effects on dynamic hyperpolarizabilities and their geometric derivatives: A comparison with density functional results. Journal of Chemical Physics, 2006, 124, 114101.	1.2	46
75	Intermolecular interaction energies by topologically partitioned electric properties II. Dispersion energies in one-centre and multicentre multipole expansions. Molecular Physics, 1997, 91, 145-160.	0.8	45
76	Coupled cluster response calculations of two-photon transition probability rate constants for helium, neon and argon. Journal of Chemical Physics, 1998, 108, 8355-8359.	1.2	43
77	Coupled cluster calculations of the frequency-dependent second hyperpolarizabilities of Ne, Ar, N <sub>2</sub> , and CH <sub>4</sub> . Journal of Chemical Physics, 1998, 109, 2762-2778.	1.2	42
78	Coupled cluster investigation of the electric-field-gradient-induced birefringence of H <sub>2</sub> , N <sub>2</sub> , C <sub>2</sub> H <sub>2</sub> , and CH <sub>4</sub> . Journal of Chemical Physics, 1998, 109, 7176-7184.	1.2	40
79	Triplet excitation energies in the coupled cluster singles and doubles model using an explicit triplet spin coupled excitation space. Journal of Chemical Physics, 2000, 113, 7765-7772.	1.2	40
80	Formation of weakly bound, ordered adlayers of CO on rutile TiO <sub>2</sub> (110): A combined experimental and theoretical study. Journal of Chemical Physics, 2009, 130, 144703.	1.2	40
81	Pair natural orbitals in explicitly correlated second-order Møller-Plesset theory. International Journal of Quantum Chemistry, 2013, 113, 224-229.	1.0	40
82	Explicitly Correlated Coupled-Cluster Theory. Challenges and Advances in Computational Chemistry and Physics, 2010, , 535-572.	0.6	40
83	OPEP: A tool for the optimal partitioning of electric properties. Journal of Computational Chemistry, 2003, 24, 997-1008.	1.5	39
84	Static and frequency-dependent polarizabilities of excited singlet states using coupled cluster response theory. Journal of Chemical Physics, 1998, 109, 9237-9243.	1.2	38
85	Ground and excited state polarizabilities and dipole transition properties of benzene from coupled cluster response theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1999, 55, 509-524.	2.0	37
86	Extensions of r12 corrections to CC2-R12 for excited states. Journal of Chemical Physics, 2006, 125, 064111.	1.2	37
87	Accuracy of Explicitly Correlated Local PNO-CCSD(T). Journal of Chemical Theory and Computation, 2017, 13, 2623-2633.	2.3	37
88	Recurrence relations for the direct calculation of spherical multipole interaction tensors and Coulomb-type interaction energies. Chemical Physics Letters, 1996, 260, 341-351.	1.2	36
89	Ab initio study of the electric-field-gradient-induced birefringence of a polar molecule: CO. Journal of Chemical Physics, 2000, 113, 3077-3087.	1.2	36
90	Sub-meV accuracy in first-principles computations of the ionization potentials and electron affinities of the atoms H to Ne. Physical Review A, 2010, 81, .	1.0	35

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91	The hyperpolarizability of the Ne atom in the approximate coupled cluster triples model CC3. <i>Chemical Physics Letters</i> , 2004, 391, 27-32.	1.2	34
92	Intermolecular interaction energies by topologically partitioned electric properties. 1. Electrostatic and induction energies in one-centre and multicentre multipole expansions. <i>Molecular Physics</i> , 1996, 88, 69-92.	0.8	34
93	Frequency-dependent nonlinear optical properties with explicitly correlated coupled-cluster response theory using the CCSD(R12) model. <i>Journal of Chemical Physics</i> , 2007, 126, 154101.	1.2	33
94	COSMO-RI-ADC(2) excitation energies and excited state gradients. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 16354-16363.	1.3	33
95	Exploring the Light-Capturing Properties of Photosynthetic Chlorophyll Clusters Using Large-Scale Correlated Calculations. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2644-2651.	2.3	32
96	The PNO- $\epsilon$ -MP2 gradient and its application to molecular geometry optimisations. <i>Molecular Physics</i> , 2017, 115, 343-356.	0.8	32
97	Derivation of coupled cluster excited states response functions and multiphoton transition moments between two excited states as derivatives of variational functionals. <i>Journal of Chemical Physics</i> , 1998, 109, 9219-9236.	1.2	31
98	Linear response CC2 triplet excitation energies. <i>Chemical Physics Letters</i> , 2000, 328, 291-301.	1.2	31
99	Quartic scaling analytical gradients of scaled opposite-spin CC2. <i>Chemical Physics</i> , 2012, 401, 217-227.	0.9	31
100	Computational screening of one- and two-photon spectrally tuned channelrhodopsin mutants. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 7567.	1.3	31
101	Ab initio calculation of the refractivity and hyperpolarizability second virial coefficients of neon gas. <i>Molecular Physics</i> , 2003, 101, 1983-1995.	0.8	30
102	Transferability of topologically partitioned polarizabilities: the case of n-alkanes. <i>Molecular Physics</i> , 1996, 89, 595-605.	0.8	29
103	Automated calculation of anharmonic vibrational contributions to first hyperpolarizabilities: Quadratic response functions from vibrational configuration interaction wave functions. <i>Journal of Chemical Physics</i> , 2009, 131, 154101.	1.2	29
104	Avoiding Electron Spill-Out in QM/MM Calculations on Excited States with Simple Pseudopotentials. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1373-1381.	2.3	29
105	TDMP2 calculation of dynamic multipole polarizabilities and dispersion coefficients of the triplebonded molecules CO, N <sub>2</sub> , CN <sup>+</sup> , and NO <sup>+</sup> . <i>Journal of Chemical Physics</i> , 1996, 105, 9948-9965.	1.2	28
106	A Density Functional Study of the Methanol Synthesis at an Oxygen Vacancy on the Polar ZnO(0001̄...) Surface. <i>Journal of Physical Chemistry C</i> , 2009, 113, 1418-1425.	1.5	28
107	Bidentate cycloimidate palladium complexes with aliphatic and aromatic anagostic bonds. <i>Chemical Communications</i> , 2014, 50, 5909.	2.2	28
108	Photophysics of the Trp-Gly dipeptide: Role of electron and proton transfer processes for efficient excited-state deactivation. <i>Chemical Physics Letters</i> , 2009, 482, 38-43.	1.2	27

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109	Large scale polarizability calculations using the approximate coupled cluster model CC2 and MP2 combined with the resolution-of-the-identity approximation. Journal of Chemical Physics, 2012, 136, 174106.	1.2	27
110	Dispersion formulas for hyperpolarizability averages. Molecular Physics, 1998, 94, 455-460.	0.8	27
111	The electric-field-gradient-induced birefringence of Helium, Neon, Argon, and SF6. Journal of Chemical Physics, 1999, 111, 7828-7836.	1.2	26
112	Optical Properties of N-Succinimidyl Bithiophene and the Effects of the Binding to Biomolecules: A Comparison between Coupled-Cluster and Time-Dependent Density Functional Theory Calculations and Experiments. Journal of Physical Chemistry B, 2006, 110, 18651-18660.	1.2	26
113	Calculation of orientation-dependent double-tensor moments for Coulomb-type intermolecular interactions. Molecular Physics, 1994, 81, 813-824.	0.8	25
114	Topologically partitioned dynamic polarizabilities using the theory of atoms in molecules. Canadian Journal of Chemistry, 1996, 74, 976-987.	0.6	25
115	A basis set study of coupled cluster and full configuration interaction calculations of molecular electric properties for BH. Chemical Physics Letters, 1998, 291, 536-546.	1.2	24
116	CC3 triplet excitation energies using an explicit spin coupled excitation space. Journal of Chemical Physics, 2001, 115, 3545-3552.	1.2	24
117	Microwave and theoretical investigation of the internal rotation in m-cresol. Journal of Chemical Physics, 2006, 124, 204305.	1.2	24
118	On the internal rotations in p-cresol in its ground and first electronically excited states. Journal of Chemical Physics, 2007, 127, 024307.	1.2	24
119	Highly accurate CCSD(R12) and CCSD(F12) optical response properties using standard triple- $\zeta$ basis sets. Journal of Chemical Physics, 2009, 131, 074102.	1.2	24
120	Investigation of interstitial hydrogen and related defects in ZnO. Physical Chemistry Chemical Physics, 2012, 14, 16392.	1.3	24
121	UV Absorption and Magnetic Circular Dichroism Spectra of Purine, Adenine, and Guanine: A Coupled Cluster Study in Vacuo and in Aqueous Solution. Journal of Chemical Theory and Computation, 2019, 15, 1242-1254.	2.3	24
122	Dispersion coefficients for first hyperpolarizabilities using coupled cluster quadratic response theory. Theoretical Chemistry Accounts, 1998, 100, 230-240.	0.5	23
123	Accurate Nonlinear Optical Properties for Small Molecules. Challenges and Advances in Computational Chemistry and Physics, 2006, , 51-99.	0.6	23
124	Comment on Quintuple- $\zeta$ quality coupled-cluster correlation energies with triple- $\zeta$ basis sets by D. P. Tew, W. Klopper, C. Neiss and C. Hättig, Phys. Chem. Chem. Phys., 2007, 9, 1921 [erratum]. Physical Chemistry Chemical Physics, 2008, 10, 6325.	1.3	23
125	Preferential pathways for light-trapping involving $\hat{I}^2$ -ligated chlorophylls. Biochimica Et Biophysica Acta - Bioenergetics, 2009, 1787, 1254-1265.	0.5	23
126	Prediction of vibrational frequencies of possible intermediates and side products of the methanol synthesis on ZnO ( $\overline{111}$ ) by <i>ab initio</i> calculations. Journal of Chemical Physics, 2012, 136, 034706.	1.2	23



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127	Coupled cluster calculations of Verdet constants. <i>Chemical Physics Letters</i> , 1997, 281, 445-451.	1.2	22
128	Femtosecond pump/probe photoelectron spectroscopy of isolated C60 negative ions. <i>Journal of Chemical Physics</i> , 2006, 125, 074312.	1.2	22
129	A combined experimental and computational study on the adsorption and reactions of NO on rutile TiO <sub>2</sub> . <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 466-472.	1.3	21
130	Response functions from Fourier component variational perturbation theory applied to a time-averaged quasienergy. <i>International Journal of Quantum Chemistry</i> , 1998, 68, 1-52.	1.0	21
131	Structures and harmonic vibrational frequencies for excited states of diatomic molecules with CCSD(R12) and CCSD(F12) models. <i>Journal of Chemical Physics</i> , 2009, 130, 124101.	1.2	19
132	The Cotton-Mouton effect of neon and argon: A benchmark study using highly correlated coupled cluster wave functions. <i>Journal of Chemical Physics</i> , 2004, 121, 9461-9473.	1.2	16
133	How Nitrogen Doping Affects Hydrogen Spillover on Carbon-Supported Pd Nanoparticles: New Insights from DFT. <i>Journal of Physical Chemistry C</i> , 2021, 125, 9020-9031.	1.5	16
134	Dispersion coefficients for second hyperpolarizabilities using coupled cluster cubic response theory. <i>Advances in Quantum Chemistry</i> , 1999, , 111-148.	0.4	15
135	Explicitly correlated second-order Møller-Plesset perturbation theory in a Divide-Expand-Consolidate (DEC) context. <i>Journal of Chemical Physics</i> , 2016, 144, 204112.	1.2	15
136	Spin-Free CC2 Implementation of Induced Transitions between Singlet Ground and Triplet Excited States. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1892-1904.	2.3	15
137	Gauge invariance of oscillator strengths in the approximate coupled cluster triples model CC3. <i>Chemical Physics Letters</i> , 2004, 389, 413-420.	1.2	14
138	Vibrational frequency scaling factors for correlation consistent basis sets and the methods CC2 and MP2 and their spin-scaled SCS and SOS variants. <i>Journal of Chemical Physics</i> , 2014, 141, 194106.	1.2	14
139	Optical rotation calculations on large molecules using the approximate coupled cluster model CC2 and the resolution-of-the-identity approximation. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 5942.	1.3	14
140	Combining Accuracy and Efficiency: An Incremental Focal-Point Method Based on Pair Natural Orbitals. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 6023-6042.	2.3	14
141	Analytic Excited State Gradients for the QM/MM Polarizable Embedded Second-Order Algebraic Diagrammatic Construction for the Polarization Propagator PE-ADC(2). <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4640-4650.	2.3	13
142	A quantum chemical study of hydrogen adsorption on carbon-supported palladium clusters. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 21577-21587.	1.3	13
143	Anchoring of palladium nanoparticles on N-doped mesoporous carbon. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 21317-21325.	1.3	13
144	Ameisensäureunterstützte selektive Hydrogenolyse von 5-Hydroxymethylfurfural zu 2,5-Dimethylfuran über bifunktionale Pd-Nanopartikel auf N-dotiertem mesoporem Kohlenstoff als Träger. <i>Angewandte Chemie</i> , 2021, 133, 6882-6891.	1.6	13

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145	Frequency-dependent hyperpolarizabilities of the Ne, Ar, and Kr atoms using the approximate coupled cluster triples model CC3. <i>Journal of Chemical Physics</i> , 2005, 123, 094303.	1.2	12
146	Density dependence of electric properties of binary mixtures of inert gases. <i>Molecular Physics</i> , 2006, 104, 305-318.	0.8	12
147	Analytic Molecular Hessian Calculations for CC2 and MP2 Combined with the Resolution of Identity Approximation. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1469-1480.	2.3	12
148	Toward assessment of density functionals for vibronic coupling in two-photon absorption: A case study of 4-nitroaniline. <i>Journal of Computational Chemistry</i> , 2015, 36, 1124-1131.	1.5	12
149	Polarizable Embedded RI-CC2 Method for Two-Photon Absorption Calculations. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3669-3678.	2.3	12
150	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)]. <i>Journal of Chemical Physics</i> , 1998, 109, 3293-3295.	1.2	11
151	The second hyperpolarizability of the N <sub>2</sub> molecule calculated using the approximate coupled cluster triples model CC3. <i>Chemical Physics Letters</i> , 2005, 413, 272-279.	1.2	11
152	Analytic Calculation of First-order Molecular Properties at the Explicitly-correlated Second-order Møller-Plesset Level. <i>Zeitschrift Fur Physikalische Chemie</i> , 2010, 224, 695-708.	1.4	11
153	Ultrafast Dynamics of a Triazene: Excited-State Pathways and the Impact of Binding to the Minor Groove of DNA and Further Biomolecular Systems. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1986-1992.	2.1	11
154	Response functions from Fourier component variational perturbation theory applied to a time-averaged quasienergy. , 1998, 68, 1.		11
155	Accurate Coupled Cluster Calculations of the Reaction Barrier Heights of Two CH <sub>3</sub> + CH <sub>4</sub> Reactions. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11679-11684.	1.1	10
156	Excited state polarizabilities for CC2 using the resolution-of-the-identity approximation. <i>Journal of Chemical Physics</i> , 2015, 143, 244108.	1.2	10
157	Magnetic circular dichroism spectra from resonant and damped coupled cluster response theory. <i>Journal of Chemical Physics</i> , 2020, 153, 114105.	1.2	10
158	Analytical nuclear gradients for electron-attached and electron-detached states for the second-order algebraic diagrammatic construction scheme combined with frozen-density embedding. <i>Journal of Chemical Physics</i> , 2020, 152, 174109.	1.2	10
159	On the calculation of derivatives for Coulomb-type interaction energies and general anisotropic pair potentials. <i>Chemical Physics Letters</i> , 1997, 268, 521-530.	1.2	9
160	Dispersion coefficients for polarizabilities and first and second hyperpolarizabilities using full configuration interaction theory. <i>Chemical Physics Letters</i> , 1999, 307, 235-243.	1.2	8
161	Theoretical Study on Noncovalent Interactions in the Carbon Nanotube-Formic Acid Dimer System. <i>Journal of Physical Chemistry C</i> , 2014, 118, 4483-4488.	1.5	8
162	Origin-independent two-photon circular dichroism calculations in coupled cluster theory. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 13683-13692.	1.3	8

#	ARTICLE	IF	CITATIONS
163	How a linear triazene photoisomerizes in a volume-conserving fashion. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 28075-28087.	1.3	8
164	Can Small Polyaromatics Describe Their Larger Counterparts for Local Reactions? A Computational Study on the H-Abstraction Reaction by an H-Atom from Polyaromatics. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9626-9637.	1.1	8
165	Structure and Reactivity of Pristine and Reduced Spinel CoFe <sub>2</sub> O <sub>4</sub> (001)/(100) Surfaces. <i>Journal of Physical Chemistry C</i> , 2021, 125, 9774-9781.	1.5	8
166	Activation of Molecular O <sub>2</sub> on CoFe <sub>2</sub> O <sub>4</sub> (001) Surfaces: An Embedded Cluster Study. <i>Chemistry - A European Journal</i> , 2021, 27, 17115-17126.	1.7	8
167	Comparison of Reaction Field Schemes for Coupling Continuum Solvation Models with Wave Function Methods for Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4554-4564.	2.3	7
168	Solvent Effects in the Ultraviolet and X-ray Absorption Spectra of Pyridazine in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 2021, 125, 7198-7206.	1.1	7
169	Magnetic Circular Dichroism of Naphthalene Derivatives: A Coupled Cluster Singles and Approximate Doubles and Time-Dependent Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2021, 125, 243-250.	1.1	7
170	Employing Pseudopotentials to Tackle Excited-State Electron Spill-Out in Frozen Density Embedding Calculations. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1737-1747.	2.3	7
171	Estimate of the experimental static hyperpolarizability of neon based on coupled cluster response calculations. <i>Chemical Physics Letters</i> , 1998, 283, 109-113.	1.2	6
172	Dispersion formulas for the second hyperpolarizability components $\hat{\beta}^3    $ , $\hat{\beta}^3 \hat{S}^2$ and $\hat{\beta}^3 K$ . <i>Chemical Physics Letters</i> , 1998, 296, 245-252.	1.2	6
173	Recent Advances in Explicitly Correlated Coupled-Cluster Response Theory for Excited States and Optical Properties. <i>Zeitschrift Fur Physikalische Chemie</i> , 2010, 224, 383-395.	1.4	6
174	Embedded cluster density functional and second-order Møller-Plesset perturbation theory study on the adsorption of N <sub>2</sub> on the rutile (110) surface. <i>Journal of Chemical Physics</i> , 2012, 137, 114705.	1.2	6
175	Implementation of the iterative triples model CC3 for excitation energies using pair natural orbitals and Laplace transformation techniques. <i>Journal of Chemical Physics</i> , 2020, 153, 034109.	1.2	6
176	Damped (linear) response theory within the resolution-of-identity coupled cluster singles and approximate doubles (RI-CC2) method. <i>Journal of Chemical Physics</i> , 2021, 154, 124110.	1.2	6
177	An automatized workflow from molecular dynamic simulation to quantum chemical methods to identify elementary reactions and compute reaction constants. <i>Journal of Computational Chemistry</i> , 2021, 42, 2264-2282.	1.5	6
178	Comment on 'Efficient calculation of canonical MP2 energies' [P. Pulay, S. Saebø, K. Wolinski, <i>Chem. Phys. Lett.</i> 344 (2001) 543-552]. <i>Chemical Physics Letters</i> , 2002, 358, 350-353.	1.2	5
179	Circularly polarised fluorescence and phosphorescence calculations on organic molecules using the approximate coupled-cluster model CC2. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 21051-21061.	1.3	5
180	Prediction of acid p <i>K<sub>a</sub></i> values in the solvent acetone based on COSMO-RS. <i>Journal of Computational Chemistry</i> , 2022, 43, 1011-1022.	1.5	4

#	ARTICLE	IF	CITATIONS
181	Cauchy Moments of Ne, Ar, and Kr Atoms Calculated Using the Approximate Coupled Cluster Triples Model CC3. <i>Advances in Quantum Chemistry</i> , 2005, , 9-21.	0.4	3
182	Anharmonic excited state frequencies of <i>para</i> -difluorobenzene, toluene and catechol using analytic RI-CC2 second derivatives. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 14063-14072.	1.3	3
183	Calculation of total photoabsorption cross sections of Ar, Kr, N2 and CO. <i>Chemical Physics</i> , 1997, 225, 309-317.	0.9	2
184	Comment on "Response to Comment on "Frequency-dependent equation-of-motion coupled cluster hyperpolarizabilities: Resolution of the discrepancy between theory and experiment for HF?â€œâ€™â€™. <i>J. Chem. Phys.</i> 109, 9201 (1998)]. <i>Journal of Chemical Physics</i> , 1998, 109, 9204-9204.		2
185	Oxidation of 2-Propanol by Peroxo Titanium Complexes: A Combined Experimental and Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2010, 114, 19415-19418.	1.5	2
186	Relaxation Dynamics of the Triazene Compound Berenil in DNA-Minor-Groove Confinement after Photoexcitation. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5203-5211.	2.3	1
187	Tracing absorption and emission characteristics of halogen-bonded ion pairs involving halogenated imidazolium species. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 7480-7494.	1.3	1
188	Analytic Calculation of First-order Molecular Properties at the Explicitly-correlated Second-order Mller-Plesset Level. , 2010, , 405-418.		0