Karol Kowalski

List of Publications by Year
in descending order

133	12,152	66315	30058
papers	citations	42	103
		h-index	g-index

134	134	134	12489
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	NWChem: A comprehensive and scalable open-source solution for large scale molecular simulations. Computer Physics Communications, 2010, 181, 1477-1489.	3.0	4,740
2	Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102.	1.2	734
3	Efficient computer implementation of the renormalized coupled-cluster methods: The R-CCSD[T], R-CCSD(T), CR-CCSD[T], and CR-CCSD(T) approaches. Computer Physics Communications, 2002, 149, 71-96.	3.0	443
4	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	1.2	425
5	The method of moments of coupled-cluster equations and the renormalized CCSD[T], CCSD(T), CCSD(TQ), and CCSDT(Q) approaches. Journal of Chemical Physics, 2000, 113, 18-35.	1.2	393
6	New coupled-cluster methods with singles, doubles, and noniterative triples for high accuracy calculations of excited electronic states. Journal of Chemical Physics, 2004, 120, 1715-1738.	1.2	301
7	The active-space equation-of-motion coupled-cluster methods for excited electronic states: Full EOMCCSDt. Journal of Chemical Physics, 2001, 115, 643-651.	1.2	261
8	Recent advances in electronic structure theory: Method of moments of coupled-cluster equations and renormalized coupled-cluster approaches. International Reviews in Physical Chemistry, 2002, 21, 527-655.	0.9	258
9	Exploiting chemistry and molecular systems for quantum information science. Nature Reviews Chemistry, 2020, 4, 490-504.	13.8	247
10	Renormalized CCSD(T) and CCSD(TQ) approaches: Dissociation of the N2 triple bond. Journal of Chemical Physics, 2000, 113, 5644-5652.	1.2	207
11	Method of moments of coupled-cluster equations: a new formalism for designing accurate electronic structure methods for ground and excited states. Theoretical Chemistry Accounts, 2004, 112, 349-393.	0.5	184
12	The active-space equation-of-motion coupled-cluster methods for excited electronic states: The EOMCCSDt approach. Journal of Chemical Physics, 2000, 113, 8490-8502.	1.2	137
13	Excited-state potential energy curves of CH+: a comparison of the EOMCCSDt and full EOMCCSDT results. Chemical Physics Letters, 2001, 347, 237-246.	1.2	120
14	Coupled Cluster Calculations of Ground and Excited States of Nuclei. Physical Review Letters, 2004, 92, 132501.	2.9	119
15	Extension of renormalized coupled-cluster methods including triple excitations to excited electronic states of open-shell molecules. Journal of Chemical Physics, 2005, 122, 214107.	1.2	113
16	New type of noniterative energy corrections for excited electronic states: Extension of the method of moments of coupled-cluster equations to the equation-of-motion coupled-cluster formalism. Journal of Chemical Physics, 2001, 115, 2966-2978.	1.2	107
17	Ab-InitioCoupled-Cluster Study ofO16. Physical Review Letters, 2005, 94, 212501.	2.9	100
18	Can ordinary single-reference coupled-cluster methods describe the potential energy curve of N2? The renormalized CCSDT(Q) study. Chemical Physics Letters, 2001, 344, 176-184.	1.2	97

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19	Extensive generalization of renormalized coupled-cluster methods. Journal of Chemical Physics, 2005, 122, 074107.	1.2	96
20	Complete set of solutions of multireference coupled-cluster equations: The state-universal formalism. Physical Review A, 2000, 61, .	1.0	87
21	Utilizing high performance computing for chemistry: parallel computational chemistry. Physical Chemistry Chemical Physics, 2010, 12, 6896.	1.3	84
22	Excited-State Studies of Polyacenes: A Comparative Picture Using EOMCCSD, CR-EOMCCSD(T), Range-Separated (LR/RT)-TDDFT, TD-PM3, and TD-ZINDO. Journal of Chemical Theory and Computation, 2011, 7, 3686-3693.	2.3	84
23	Accurate dipole polarizabilities for water clusters n=2â€“12 at the coupled-cluster level of theory and benchmarking of various density functionals. Journal of Chemical Physics, 2009, 131, 214103.	1.2	83
24	Extension of the method of moments of coupled-cluster equations to a multireference wave operator formalism. Computational and Theoretical Chemistry, 2001, 547, 191-208.	1.5	82
25	Extension of the method of moments of coupled-cluster equations to excited states: The triples and quadruples corrections to the equation-of-motion coupled-cluster singles and doubles energies. Journal of Chemical Physics, 2002, 116, 7411-7423.	1.2	81
26	In Search of the Relationship between Multiple Solutions Characterizing Coupled-Cluster Theories. Computational Chemistry - Reviews of Current Trends, 2000, , 1-104.	0.4	75
27	Charge-Transfer Versus Charge-Transfer-Like Excitations Revisited. Journal of Chemical Theory and Computation, 2015, 11, 3305-3320.	2.3	75
28	GPU-Based Implementations of the Noniterative Regularized-CCSD(T) Corrections: Applications to Strongly Correlated Systems. Journal of Chemical Theory and Computation, 2011, 7, 1316-1327.	2.3	72
29	Hybrid approach for free energy calculations with high-level methods: Application to the SN2 reaction of CHCl3 and OHâ^' in water. Journal of Chemical Physics, 2007, 127, 051102.	1.2	70
30	Modeling Excited States in TiO₂ Nanoparticles: On the Accuracy of a TD-DFT Based Description. Journal of Chemical Theory and Computation, 2014, 10, 1189-1199.	2.3	63
31	Comparison of low-order multireference many-body perturbation theories. Journal of Chemical Physics, 2005, 122, 134105.	1.2	62
32	Electronic Structure and Stability of [B₁₂X₁₂]^{2â€“} (X = Fâ€“At): A Combined Photoelectron Spectroscopic and Theoretical Study. Journal of the American Chemical Society, 2017, 139, 14749-14756.	6.6	60
33	Active-space coupled-cluster study of electronic states of Be3. Journal of Chemical Physics, 2005, 123, 074319.	1.2	59
34	Active-space completely-renormalized equation-of-motion coupled-cluster formalism: Excited-state studies of green fluorescent protein, free-base porphyrin, and oligoporphyrin dimer. Journal of Chemical Physics, 2010, 132, 154103.	1.2	59
35	New classes of non-iterative energy corrections to multi-reference coupled-cluster energies. Molecular Physics, 2004, 102, 2425-2449.	0.8	58
36	Downfolding of many-body Hamiltonians using active-space models: Extension of the sub-system embedding sub-algebras approach to unitary coupled cluster formalisms. Journal of Chemical Physics, 2019, 151, 014107.	1.2	57

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37	Can ordinary single-reference coupled-cluster methods describe potential energy surfaces with nearly spectroscopic accuracy? The renormalized coupled-cluster study of the vibrational spectrum of HF. Journal of Chemical Physics, 2001, 115, 5796-5804.	1.2	53
38	Automated derivation and parallel computer implementation of renormalized and active-space coupled-cluster methods. International Journal of Quantum Chemistry, 2006, 106, 79-97.	1.0	53
39	Hybrid coupled cluster and molecular dynamics approach: Application to the excitation spectrum of cytosine in the native DNA environment. Journal of Chemical Physics, 2006, 125, 211101.	1.2	51
40	Resource-Efficient Chemistry on Quantum Computers with the Variational Quantum Eigensolver and the Double Unitary Coupled-Cluster Approach. Journal of Chemical Theory and Computation, 2020, 16, 6165-6175.	2.3	50
41	Dynamic polarizabilities of polyaromatic hydrocarbons using coupled-cluster linear response theory. Journal of Chemical Physics, 2007, 127, 144105.	1.2	49
42	Large-scale parallel calculations with combined coupled cluster and molecular mechanics formalism: Excitation energies of zincâ€“porphyrin in aqueous solution. Chemical Physics Letters, 2008, 458, 205-209.	1.2	46
43	Exactness of Two-Body Cluster Expansions in Many-Body Quantum Theory. Physical Review Letters, 2003, 90, 113001.	2.9	43
44	Coupled cluster calculations for static and dynamic polarizabilities of C60. Journal of Chemical Physics, 2008, 129, 226101.	1.2	43
45	Communication: Application of state-specific multireference coupled cluster methods to core-level excitations. Journal of Chemical Physics, 2012, 137, 171101.	1.2	42
46	Coupled cluster Green function: Model involving single and double excitations. Journal of Chemical Physics, 2016, 144, 144101.	1.2	42
47	Highly Efficient and Scalable Compound Decomposition of Two-Electron Integral Tensor and Its Application in Coupled Cluster Calculations. Journal of Chemical Theory and Computation, 2017, 13, 4179-4192.	2.3	41
48	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. Chemical Reviews, 2021, 121, 4962-4998.	23.0	39
49	Complete set of solutions of the generalized Bloch equation. International Journal of Quantum Chemistry, 2000, 80, 757-781.	1.0	38
50	Noniterative Multireference Coupled Cluster Methods on Heterogeneous CPUâ€“GPU Systems. Journal of Chemical Theory and Computation, 2013, 9, 1949-1957.	2.3	37
51	Coupled-cluster representation of Green function employing modified spectral resolutions of similarity transformed Hamiltonians. Journal of Chemical Physics, 2014, 141, 094102.	1.2	35
52	Renormalized coupled-cluster calculations of reactive potential energy surfaces: A comparison of the CCSD(T), renormalized CCSD(T), and full configuration interaction results for the collinear BeFH system. Journal of Chemical Physics, 2002, 117, 3617-3624.	1.2	34
53	Describing Excited State Relaxation and Localization in TiO₂ Nanoparticles Using TD-DFT. Journal of Chemical Theory and Computation, 2014, 10, 5538-5548.	2.3	34
54	Properties of coupled-cluster equations originating in excitation sub-algebras. Journal of Chemical Physics, 2018, 148, .	1.2	34

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55	Optimizing tensor contraction expressions for hybrid CPU-GPU execution. Cluster Computing, 2013, 16, 131-155.	3.5	32
56	Greenâ€™s Function Coupled-Cluster Approach: Simulating Photoelectron Spectra for Realistic Molecular Systems. Journal of Chemical Theory and Computation, 2018, 14, 4335-4352.	2.3	32
57	Optimization of the Coupled Cluster Implementation in NWChem on Petascale Parallel Architectures. Journal of Chemical Theory and Computation, 2014, 10, 4307-4316.	2.3	31
58	Method of moments of coupled-cluster equations: The quasivariational and quadratic approximations. Journal of Chemical Physics, 2003, 119, 2951-2962.	1.2	29
59	Implementation of the locally renormalized CCSD(T) approaches for arbitrary reference function. Journal of Chemical Physics, 2005, 123, 014102.	1.2	29
60	Physical and mathematical content of coupled-cluster equations. IV. Impact of approximations to the cluster operator on the structure of solutions. Journal of Chemical Physics, 1999, 111, 2952-2959.	1.2	27
61	Method of Moments of Coupled-Cluster Equations: A New Theoretical Framework for Designing "Black-Box" Approaches for Molecular Potential Energy Surfaces. ACS Symposium Series, 2002, , 31-64.	0.5	26
62	Visible Light Absorption of N-Doped TiO₂ Rutile Using (LR/RT)-TDDFT and Active Space EOMCCSD Calculations. Journal of Physical Chemistry Letters, 2011, 2, 2696-2701.	2.1	26
63	A universal state-selective approach to multireference coupled-cluster non-iterative corrections. Journal of Chemical Physics, 2011, 134, 194107.	1.2	26
64	Parallel Implementation of Multireference Coupled-Cluster Theories Based on the Reference-Level Parallelism. Journal of Chemical Theory and Computation, 2012, 8, 487-497.	2.3	25
65	Coupled-cluster Green's function: Analysis of properties originating in the exponential parametrization of the ground-state wave function. Physical Review A, 2016, 94, .	1.0	25
66	Quantum simulations of excited states with active-space downfolded Hamiltonians. Journal of Chemical Physics, 2019, 151, 234114.	1.2	25
67	Sub-system quantum dynamics using coupled cluster downfolding techniques. Journal of Chemical Physics, 2020, 152, 244127.	1.2	25
68	Equation of motion coupled-cluster cumulant approach for intrinsic losses in x-ray spectra. Journal of Chemical Physics, 2020, 152, 174113.	1.2	25
69	Physical and mathematical content of coupledâ€“cluster equations: Correspondence between coupledâ€“cluster and configurationâ€“interaction solutions. Journal of Chemical Physics, 1999, 110, 3714-3729.	1.2	24
70	Scalable implementations of accurate excited-state coupled cluster theories. , 2011, , .		24
71	Benchmarking the Fundamental Electronic Properties of small TiO₂ Nanoclusters by GW and Coupled Cluster Theory Calculations. Journal of Chemical Theory and Computation, 2017, 13, 3814-3828.	2.3	24
72	Physical and mathematical content of coupled-cluster equations. II. On the origin of irregular solutions and their elimination via symmetry adaptation. Journal of Chemical Physics, 1999, 110, 9345-9352.	1.2	22

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73	Role of Many-Body Effects in Describing Low-Lying Excited States of Ï€-Conjugated Chromophores: High-Level Equation-of-Motion Coupled-Cluster Studies of Fused Porphyrin Systems. Journal of Chemical Theory and Computation, 2011, 7, 2200-2208.	2.3	22
74	Massively parallel implementation of the multireference Brillouinâ€“Wigner CCSD method. Chemical Physics Letters, 2011, 514, 347-351.	1.2	22
75	Efficient Implementation of Many-Body Quantum Chemical Methods on the Intel® Xeon Phi Coprocessor. , 2014, , .		22
76	Universal state-selective corrections to multi-reference coupled-cluster theories with single and double excitations. Journal of Chemical Physics, 2012, 136, 124102.	1.2	21
77	Physical and mathematical content of coupled-cluster equations. III. Model studies of dissociation processes for various reference states. Journal of Chemical Physics, 1999, 111, 2940-2951.	1.2	20
78	Implementation of the multireference Brillouin-Wigner and Mukherjee's coupled cluster methods with non-iterative triple excitations utilizing reference-level parallelism. Journal of Chemical Physics, 2012, 137, 094112.	1.2	19
79	Real-Time Coupled-Cluster Approach for the Cumulant Greenâ€™s Function. Journal of Chemical Theory and Computation, 2020, 16, 6983-6992.	2.3	19
80	Multiple solutions of the single-reference coupled-cluster equations. I. H4 model revisited. International Journal of Quantum Chemistry, 1994, 50, 353-367.	1.0	18
81	Approximate coupled-cluster methods employing split cluster amplitudes: Implementation of an almost-linear coupled-cluster formalism. Journal of Chemical Physics, 1998, 109, 6255-6263.	1.2	18
82	Multiple solutions of the single-reference coupled-cluster equations. II. Alternative reference states. International Journal of Quantum Chemistry, 1995, 53, 501-514.	1.0	17
83	Approximate Greenâ€™s Function Coupled Cluster Method Employing Effective Dimension Reduction. Journal of Chemical Theory and Computation, 2019, 15, 3185-3196.	2.3	17
84	Quantum simulations employing connected moments expansions. Journal of Chemical Physics, 2020, 153, 201102.	1.2	17
85	Dimensionality reduction of the many-body problem using coupled-cluster subsystem flow equations: Classical and quantum computing perspective. Physical Review A, 2021, 104, .	1.0	17
86	Equation of motion coupled cluster methods for electron attachment and ionization potential in fullerenes C60and C70. Journal of Chemical Physics, 2014, 141, 074304.	1.2	16
87	Properties of advanced coupled-cluster Green's function. Molecular Physics, 2018, 116, 561-569.	0.8	16
88	Toward Quantum Computing for High-Energy Excited States in Molecular Systems: Quantum Phase Estimations of Core-Level States. Journal of Chemical Theory and Computation, 2021, 17, 201-210.	2.3	16
89	Towards large-scale calculations with State-Specific Multireference Coupled Cluster methods: Studies on dodecane, naphthynes, and polycarbenes. Chemical Physics Letters, 2012, 542, 128-133.	1.2	13
90	Coupled cluster calculations on TiO2 nanoclusters. Journal of Chemical Physics, 2013, 139, 064313.	1.2	13

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91	Theoretical studies of the global minima and polarizabilities of small lithium clusters. Chemical Physics Letters, 2016, 644, 235-242.	1.2	13
92	Equation of motion coupled cluster methods for electron attachment and ionization potential in polyacenes. Chemical Physics Letters, 2015, 641, 146-152.	1.2	12
93	Linear response coupled cluster singles and doubles approach with modified spectral resolution of the similarity transformed Hamiltonian. Journal of Chemical Physics, 2007, 127, 164105.	1.2	11
94	Toward Enabling Large-Scale Open-Shell Equation-of-Motion Coupled Cluster Calculations: Triplet States of Î²-Carotene. Journal of Physical Chemistry A, 2014, 118, 9087-9093.	1.1	11
95	Greenâ€™s function coupled cluster formulations utilizing extended inner excitations. Journal of Chemical Physics, 2018, 149, 214102.	1.2	11
96	Variational quantum solver employing the PDS energy functional. Quantum - the Open Journal for Quantum Science, 0, 5, 473.	0.0	11
97	Improving the accuracy and efficiency of quantum connected moments expansions *. Quantum Science and Technology, 2021, 6, 034012.	2.6	11
98	Coupled Cluster Downfolding Theory: towards universal many-body algorithms for dimensionality reduction of composite quantum systems in chemistry and materials science. Materials Theory, 2022, 6, .	2.2	11
99	Model study of the impact of orbital choice on the accuracy of coupled-cluster energies. I. Single-reference-state formulation. International Journal of Quantum Chemistry, 1998, 67, 205-219.	1.0	10
100	Toward generalized tensor algebra for ab initio quantum chemistry methods. , 2019, , .		10
101	Quantum Solvers for Plane-Wave Hamiltonians: Abridging Virtual Spaces Through the Optimization of Pairwise Correlations. Frontiers in Chemistry, 2021, 9, 603019.	1.8	10
102	Real-Time Equation-of-Motion CCSD Cumulant Greenâ€™s Function. Journal of Chemical Theory and Computation, 2022, 18, 1799-1807.	2.3	10
103	Coupled Cluster Studies of Ionization Potentials and Electron Affinities of Single-Walled Carbon Nanotubes. Journal of Physical Chemistry A, 2017, 121, 1328-1335.	1.1	9
104	Coupled Cluster Downfolding Methods: the effect of double commutator terms on the accuracy of ground-state energies. Journal of Chemical Physics, 2022, 156, 094106.	1.2	9
105	Advances in Scalable Computational Chemistry. Annual Reports in Computational Chemistry, 2011, 7, 151-177.	0.9	8
106	Note: Excited state studies of ozone using state-specific multireference coupled cluster methods. Journal of Chemical Physics, 2012, 137, 216101.	1.2	8
107	GFCCLib: Scalable and efficient coupled-cluster Green's function library for accurately tackling many-body electronic structure problems. Computer Physics Communications, 2021, 265, 108000.	3.0	8
108	Equation-of-Motion Coupled-Cluster Cumulant Greenâ€™s Function for Excited States and X-Ray Spectra. Frontiers in Chemistry, 2021, 9, 734945.	1.8	8

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109	New Alternatives for Accurate Electronic Structure Calculations of Potential Energy Surfaces Involving Bond Breaking. ACS Symposium Series, 2007, , 37-73.	0.5	7
110	Effective Utilization of Tensor Symmetry in Operation Optimization of Tensor Contraction Expressions. Procedia Computer Science, 2012, 9, 412-421.	1.2	7
111	Implementation of High-Order Multireference Coupled-Cluster Methods on Intel Many Integrated Core Architecture. Journal of Chemical Theory and Computation, 2016, 12, 1129-1138.	2.3	7
112	Low-rank factorization of electron integral tensors and its application in electronic structure theory. Chemical Physics Letters, 2017, 672, 47-53.	1.2	7
113	A MRCC study of the isomerisation of cyclopropane. Molecular Physics, 2017, 115, 2743-2754.	0.8	7
114	Bridging single and multireference coupled cluster theories with universal state selective formalism. Journal of Chemical Physics, 2013, 138, 204114.	1.2	6
115	Iterative universal state selective correction for the Brillouin-Wigner multireference coupled-cluster theory. Journal of Chemical Physics, 2015, 142, 114106.	1.2	6
116	Perturbative universal state-selective correction for state-specific multi-reference coupled cluster methods. Journal of Chemical Physics, 2016, 145, 164106.	1.2	6
117	Greenâ€™s function coupled cluster simulation of the near-valence ionizations of DNA-fragments. Journal of Chemical Physics, 2020, 152, 011101.	1.2	6
118	Solving Coupled Cluster Equations by the Newton Krylov Method. Frontiers in Chemistry, 2020, 8, 590184.	1.8	6
119	Coupled cluster Green's function: Past, present, and future. Annual Reports in Computational Chemistry, 2021, , 23-53.	0.9	6
120	Coupled Cluster Green's function formulations based on the effective Hamiltonians. Molecular Physics, 2020, 118, e1725669.	0.8	5
121	Transitioning NWChem to the Next Generation of Manycore Machines. , 2017, , 165-186.		5
122	Correspondence between physical states and solutions to the coupled-cluster equations. , 1999, 75, 483-496.		4
123	Regularized and Renormalized Many-Body Techniques for Describing Correlated Molecular Systems: A Coupled-Cluster Perspective. Annual Reports in Computational Chemistry, 2018, 14, 3-45.	0.9	4
124	Real-time equation-of-motion CC cumulant and CC Greenâ€™s function simulations of photoemission spectra of water and water dimer. Journal of Chemical Physics, 2022, 157, .	1.2	4
125	Excitation transfer between the rubidium52Dfine-structure levels in collisions with ground-state rubidium atoms: Experiment and theory. Physical Review A, 2000, 62, .	1.0	3
126	Ab initio coupled cluster calculations for nuclei using methods of quantum chemistry. European Physical Journal A, 2005, 25, 485-488.	1.0	3

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127	Scalable Heterogeneous Execution of a Coupled-Cluster Model with Perturbative Triples. , 2020, , .		3
128	Hybrid quantum-classical approach for coupled-cluster Green's function theory. Quantum - the Open Journal for Quantum Science, 0, 6, 675.	0.0	3
129	The role of a dipole-coupled but not dipole-probed state in probe absorption with multilevel coupling. European Physical Journal: Special Topics, 2013, 222, 2197-2206.	1.2	2
130	Accelerating the Global Arrays ComEx Runtime Using Multiple Progress Ranks. , 2019, , .		2
131	Cross Sections for l-Mixing of K(n²F) States in Collisions with Ground-State K(4²S) Atoms. Acta Physica Polonica A, 2000, 98, 353-361.	0.2	2
132	Complete set of solutions of the generalized Bloch equation. International Journal of Quantum Chemistry, 2000, 80, 757-781.	1.0	1
133	COUPLED CLUSTER APPROACHES TO NUCLEI, GROUND STATES AND EXCITED STATES. , 2005, , .		0