Piotr Piecuch

List of Publications by Year
in descending order

232 papers	13,474 citations	18482 62 h-index	25787 108 g-index
241 all docs	241 docs citations	241 times ranked	4270 citing authors

#	Article	IF	Citations
1	Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102.	3.0	734
2	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.	7.5	443
3	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.	3.0	393
4	Renormalized coupled-cluster methods exploiting left eigenstates of the similarity-transformed Hamiltonian. Journal of Chemical Physics, 2005, 123, 224105.	3.0	391
5	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.	3.0	301
6	A stateâ€selective multireference coupledâ€cluster theory employing the singleâ€reference formalism. Journal of Chemical Physics, 1993, 99, 1875-1900.	3.0	300
7	The active-space equation-of-motion coupled-cluster methods for excited electronic states: Full EOMCCSDt. Journal of Chemical Physics, 2001, 115, 643-651.	3.0	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.	2.3	258
9	Coupled-cluster methods with internal and semi-internal triply and quadruply excited clusters: CCSDt and CCSDtq approaches. Journal of Chemical Physics, 1999, 110, 6103-6122.	3.0	228
10	Application of Hilbert-space coupled-cluster theory to simple (H2)2model systems: Planar models. Physical Review A, 1993, 47, 2738-2782.	2.5	217
11	Renormalized CCSD(T) and CCSD(TQ) approaches: Dissociation of the N2 triple bond. Journal of Chemical Physics, 2000, 113, 5644-5652.	3.0	207
12	Where Does the Planar-to-Nonplanar Turnover Occur in Small Gold Clusters?. Journal of the American Chemical Society, 2005, 127, 1049-1052.	13.7	207
13	Local correlation calculations using standard and renormalized coupled-cluster approaches. Journal of Chemical Physics, 2009, 131, 114109.	3.0	199
14	Stateâ€selective multireference coupledâ€cluster theory employing the singleâ€reference formalism: Implementation and application to the H8 model system. Journal of Chemical Physics, 1994, 100, 5792-5809.	3.0	192
15	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.	1.4	184
16	Single-reference, size-extensive, non-iterative coupled-cluster approaches to bond breaking and biradicals. Chemical Physics Letters, 2006, 418, 467-474.	2.6	180
17	Theoretical Models on the Cu2O2 Torture Track:â€‰ Mechanistic Implications for Oxytyrosinase and Small-Molecule Analogues. Journal of Physical Chemistry A, 2006, 110, 1991-2004.	2.5	179
18	Extension of the Renormalized Coupled-Cluster Methods Exploiting Left Eigenstates of the Similarity-Transformed Hamiltonian to Open-Shell Systems:â€‰ A Benchmark Study. Journal of Physical Chemistry A, 2007, 111, 11359-11382.	2.5	178

#	Article	IF	Citations
19	Combined coupled-cluster and many-body perturbation theories. Journal of Chemical Physics, 2004, 121, 12197.	3.0	161
20	Coupled-cluster theory for three-body Hamiltonians. Physical Review C, 2007, 76, .	2.9	147
21	A comparison of the renormalized and active-space coupled-cluster methods: Potential energy curves of BH and F2. Chemical Physics Letters, 2001, 344, 165-175.	2.6	138
22	The active-space equation-of-motion coupled-cluster methods for excited electronic states: The EOMCCSDt approach. Journal of Chemical Physics, 2000, 113, 8490-8502.	3.0	137
23	Excited-state potential energy curves of CH+: a comparison of the EOMCCSDt and full EOMCCSDT results. Chemical Physics Letters, 2001, 347, 237-246.	2.6	120
24	Coupled Cluster Calculations of Ground and Excited States of Nuclei. Physical Review Letters, 2004, 92, 132501.	7.8	119
25	Orthogonally spin-adapted coupled-cluster equations involving singly and doubly excited clusters. Comparison of different procedures for spin-adaptation. International Journal of Quantum Chemistry, 1989, 36, 429-453.	2.0	118
26	Orthogonally spin-adapted multi-reference Hilbert space coupled-cluster formalism: diagrammatic formulation. Theoretica Chimica Acta, 1992, 83, 69-103.	0.8	117
27	Approximate account of connected quadruply excited clusters in single-reference coupled-cluster theory via cluster analysis of the projected unrestricted Hartree-Fock wave function. Physical Review A, 1996, 54, 1210-1241.	2.5	115
28	Thermochemical Kinetics for Multireference Systems: Addition Reactions of Ozone. Journal of Physical Chemistry A, 2009, 113, 5786-5799.	2.5	114
29	Application of Hilbert-space coupled-cluster theory to simple (H2)2model systems. II. Nonplanar models. Physical Review A, 1994, 49, 3479-3514.	2.5	113
30	Extension of renormalized coupled-cluster methods including triple excitations to excited electronic states of open-shell molecules. Journal of Chemical Physics, 2005, 122, 214107.	3.0	113
31	Orthogonally spinâ€adapted stateâ€universal coupledâ€cluster formalism: Implementation of the complete twoâ€reference theory including cubic and quartic coupling terms. Journal of Chemical Physics, 1994, 101, 5875-5890.	3.0	112
32	Leftâ€eigenstate completely renormalized equationâ€ofâ€motion coupledâ€cluster methods: Review of key concepts, extension to excited states of openâ€shell systems, and comparison with electronâ€attached and ionized approaches. International Journal of Quantum Chemistry, 2009, 109, 3268-3304.	2.0	110
33	Two new classes of non-iterative coupled-cluster methods derived from the method of moments of coupled-cluster equations. Molecular Physics, 2006, 104, 2149-2172.	1.7	108
34	Coupled cluster approaches with an approximate account of triexcitations and the optimized inner projection technique. Theoretica Chimica Acta, 1990, 78, 65-128.	0.8	107
35	EOMXCC: A New Coupled-Cluster Method for Electronic Excited States. Advances in Quantum Chemistry, 1999, 34, 295-380.	0.8	107
36	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.	3.0	107

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37	Multilevel Extension of the Cluster-in-Molecule Local Correlation Methodology: Merging Coupled-Cluster and MÃ¸llerâ"Plesset Perturbation Theories. Journal of Physical Chemistry A, 2010, 114, 6721-6727.	2.5	107
38	Active-space equation-of-motion coupled-cluster methods for excited states of radicals and other open-shell systems: EA-EOMCCSDt and IP-EOMCCSDt. Journal of Chemical Physics, 2005, 123, 134113.	3.0	103
39	Ab-InitioCoupled-Cluster Study ofO16. Physical Review Letters, 2005, 94, 212501.	7.8	100
40	The XÎ£g+1, BÎ"g1, and Bâ€²Î£g+1 states of C2: A comparison of renormalized coupled-cluster and multireference methods with full configuration interaction benchmarks. Journal of Chemical Physics, 2005, 122, 124104.	3.0	99
41	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.	2.6	97
42	The Cobaltâ€"Methyl Bond Dissociation in Methylcobalamin: New Benchmark Analysis Based on Density Functional Theory and Completely Renormalized Coupled-Cluster Calculations. Journal of Chemical Theory and Computation, 2012, 8, 1870-1894.	5.3	97
43	Extensive generalization of renormalized coupled-cluster methods. Journal of Chemical Physics, 2005, 122, 074107.	3.0	96
44	Improved computational strategy for the stateâ€selective coupledâ€cluster theory with semiâ€internal triexcited clusters: Potential energy surface of the HF molecule. Journal of Chemical Physics, 1995, 103, 9331-9346.	3.0	95
45	Efficient formulation and computer implementation of the active-space electron-attached and ionized equation-of-motion coupled-cluster methods. Journal of Chemical Physics, 2006, 125, 234107.	3.0	92
46	Improved Design of Orbital Domains within the Cluster-in-Molecule Local Correlation Framework: Single-Environment Cluster-in-Molecule Ansatz and Its Application to Local Coupled-Cluster Approach with Singles and Doubles^{â€}. Journal of Physical Chemistry A, 2010, 114, 8644-8657.	2.5	91
47	The Ground State Electronic Energy of Benzene. Journal of Physical Chemistry Letters, 2020, 11, 8922-8929.	4.6	90
48	Complete set of solutions of multireference coupled-cluster equations: The state-universal formalism. Physical Review A, 2000, 61, .	2.5	87
49	Coupled-cluster methods with internal and semi-internal triply excited clusters: Vibrational spectrum of the HF molecule. Journal of Chemical Physics, 1999, 111, 6679-6692.	3.0	86
50	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
51	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.	3.0	81
52	Theoretical Characterization of End-On and Side-On Peroxide Coordination in Ligated Cu2O2 Models. Journal of Physical Chemistry A, 2006, 110, 11557-11568.	2.5	80
53	Active-space coupled-cluster methods. Molecular Physics, 2010, 108, 2987-3015.	1.7	80
54	Molecular quadrupole moment functions of HF and N2. I.Abinitiolinearâ€response coupledâ€cluster results. Journal of Chemical Physics, 1996, 104, 4699-4715.	3.0	79

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55	In Search of the Relationship between Multiple Solutions Characterizing Coupled-Cluster Theories. Computational Chemistry - Reviews of Current Trends, 2000, , 1-104.	0.4	75
56	Converging High-Level Coupled-Cluster Energetics by MonteÂCarlo Sampling and Moment Expansions. Physical Review Letters, 2017, 119, 223003.	7.8	73
57	Doubly electron-attached and doubly ionized equation-of-motion coupled-cluster methods with 4-particleâ€“2-hole and 4-holeâ€“2-particle excitations and their active-space extensions. Journal of Chemical Physics, 2013, 138, 194102.	3.0	71
58	Biorthogonal moment expansions in coupled-cluster theory: Review of key concepts and merging the renormalized and active-space coupled-cluster methods. Chemical Physics, 2012, 401, 180-202.	1.9	69
59	Breaking bonds with the stateâ€selective multireference coupledâ€cluster method employing the singleâ€reference formalism. Journal of Chemical Physics, 1995, 102, 898-904.	3.0	68
60	Coupled-cluster approaches with an approximate account of triexcitations and the optimized-inner-projection technique. II. Coupled-cluster results for cyclic-polyene model systems. Physical Review B, 1990, 42, 3351-3379.	3.2	65
61	Coupled-cluster calculations for valence systems aroundO16. Physical Review C, 2006, 74, .	2.9	64
62	Breaking bonds with the left eigenstate completely renormalized coupled-cluster method. Journal of Chemical Physics, 2007, 127, 174106.	3.0	63
63	Embedding vs Supermolecular Strategies in Evaluating the Hydrogen-Bonding-Induced Shifts of Excitation Energies. Journal of Chemical Theory and Computation, 2011, 7, 1647-1666.	5.3	63
64	Comparison of low-order multireference many-body perturbation theories. Journal of Chemical Physics, 2005, 122, 134105.	3.0	62
65	Communication: Approaching exact quantum chemistry by cluster analysis of full configuration interaction quantum Monte Carlo wave functions. Journal of Chemical Physics, 2018, 149, 151101.	3.0	62
66	Combining active-space coupled-cluster methods with moment energy corrections via the CC(P;Q) methodology, with benchmark calculations for biradical transition states. Journal of Chemical Physics, 2012, 136, 144104.	3.0	61
67	Method of moments approach and coupled cluster theory. Theoretica Chimica Acta, 1991, 80, 223-243.	0.8	60
68	Photoluminescence, photophysics, and photochemistry of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:msub><mml:mi mathvariant="normal">V</mml:mi><mml:mi mathvariant="normal">B</mml:mi></mml:msub></mml:mrow><mml:mo>â^’</mml:mo></mml:msup></mml:math> defect in hexagonal boron nitride. Physical Review B, 2020, 102, .	3.2	60
69	Potential energy surfaces of NaFH. Journal of Chemical Physics, 1998, 108, 5349-5377.	3.0	59
70	Active-space coupled-cluster study of electronic states of Be3. Journal of Chemical Physics, 2005, 123, 074319.	3.0	59
71	New classes of non-iterative energy corrections to multi-reference coupled-cluster energies. Molecular Physics, 2004, 102, 2425-2449.	1.7	58
72	Stereoelectronic Effects on Molecular Geometries and State-Energy Splittings of Ligated Monocopper Dioxygen Complexes. Journal of Physical Chemistry A, 2008, 112, 3754-3767.	2.5	58

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73	The state-selective coupled cluster method for quasi-degenerate electronic states. Molecular Physics, 1998, 94, 225-234.	1.7	57
74	State-selective multi-reference coupled-cluster theory using multi-configuration self-consistent-field orbitals. A model study on H8. Chemical Physics Letters, 1994, 221, 121-128.	2.6	56
75	Stateâ€selective multireference coupledâ€cluster theory: In pursuit of property calculation. Journal of Chemical Physics, 1996, 104, 6582-6589.	3.0	56
76	Balancing Dynamic and Nondynamic Correlation for Diradical and Aromatic Transition States:Â A Renormalized Coupled-Cluster Study of the Cope Rearrangement of 1,5-Hexadiene. Journal of the American Chemical Society, 2005, 127, 2608-2614.	13.7	56
77	A study of 1A1-3B1 separation in CH2 using orthogonally spin-adapted state-universal and state-specific coupled-cluster methods. Chemical Physics Letters, 1994, 224, 267-274.	2.6	55
78	Orthogonally spinâ€adapted singleâ€reference coupledâ€cluster formalism: Linear response calculation of static properties. Journal of Chemical Physics, 1995, 102, 6511-6524.	3.0	55
79	The State-Universal Multi-Reference Coupled-Cluster Theory: An Overview of Some Recent Advances. International Journal of Molecular Sciences, 2002, 3, 676-709.	4.1	55
80	Extension of coupled-cluster theory with a noniterative treatment of connected triply excited clusters to three-body Hamiltonians. Physical Review C, 2013, 88, .	2.9	55
81	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.	3.0	53
82	Automated derivation and parallel computer implementation of renormalized and active-space coupled-cluster methods. International Journal of Quantum Chemistry, 2006, 106, 79-97.	2.0	53
83	Merging Active-Space and Renormalized Coupled-Cluster Methods via the CC(P;Q) Formalism, with Benchmark Calculations for Singletâ€“Triplet Gaps in Biradical Systems. Journal of Chemical Theory and Computation, 2012, 8, 4968-4988.	5.3	53
84	Electronic structure of the S₁ state in methylcobalamin: Insight from CASSCF/MCâ€XQDPT2, EOMâ€CCSD, and TDâ€DFT calculations. Journal of Computational Chemistry, 2013, 34, 987-1004.	3.3	53
85	Approximate account of connected quadruply excited clusters in multi-reference Hilbert space coupled-cluster theory. Application to planar H4 models. Chemical Physics Letters, 1993, 210, 243-252.	2.6	51
86	Experimental and Theoretical UV Characterizations of Acetylacetone and Its Isomers. Journal of Physical Chemistry A, 2006, 110, 3920-3926.	2.5	51
87	Solving the singleâ€reference coupledâ€cluster equations involving highly excited clusters in quasidegenerate situations. Journal of Chemical Physics, 1994, 100, 5857-5869.	3.0	50
88	Orthogonally spinâ€adapted singleâ€reference coupledâ€cluster formalism: Linear response calculation of higherâ€order static properties. Journal of Chemical Physics, 1996, 104, 8566-8585.	3.0	50
89	Non-iterative corrections to extended coupled-cluster energies employing the generalized method of moments of coupled-cluster equations. Molecular Physics, 2005, 103, 2191-2213.	1.7	50
90	Computational Investigation of the Conrotatory and Disrotatory Isomerization Channels of Bicyclo[1.1.0]butane to Buta-1,3-diene:Â A Completely Renormalized Coupled-Cluster Study. Journal of Physical Chemistry A, 2007, 111, 734-742.	2.5	49

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91	The nonadditive interactions in the Ar2HF and Ar2HCl clusters: An ab initio study. Journal of Chemical Physics, 1993, 99, 6732-6741.	3.0	48
92	Coupled-Cluster approaches with an approximate account of triply and quadruply excited clusters: Implementation of the orthogonally spin-adaptedCCD +ST(CCD),CCSD +T(CCSD), andACPQ +ST(ACPQ) formalisms. International Journal of Quantum Chemistry, 1995, 55, 133-146.	2.0	48
93	Photodissociation of LiFH and NaFH van der Waals complexes: A semiclassical trajectory study. Journal of Chemical Physics, 2001, 115, 7945-7952.	3.0	46
94	The photoabsorption spectrum of Naâ‹¯FH van der Waals molecule: Comparison of theory and experiment for a harpooning reaction studied by transition state spectroscopy. Journal of Chemical Physics, 1998, 108, 5378-5390.	3.0	45
95	Active-space symmetry-adapted-cluster configuration-interaction and equation-of-motion coupled-cluster methods for high accuracy calculations of potential energy surfaces of radicals. Journal of Chemical Physics, 2007, 126, 164111.	3.0	45
96	Electron correlation in one dimension: Coupled cluster approaches to cyclic polyene ?-electron models. International Journal of Quantum Chemistry, 1992, 42, 135-164.	2.0	43
97	An ab initio determination of 1A1-3B1 energy gap in CH2 using orthogonally spin-adapted state-universal and state-specific coupled-cluster methods. Chemical Physics Letters, 1994, 230, 377-386.	2.6	43
98	Exactness of Two-Body Cluster Expansions in Many-Body Quantum Theory. Physical Review Letters, 2003, 90, 113001.	7.8	43
99	The Usefulness of Exponential Wave Function Expansions Employing One- and Two-Body Cluster Operators in Electronic Structure Theory: The Extended and Generalized Coupled-Cluster Methods. Advances in Quantum Chemistry, 2006, 51, 1-57.	0.8	43
100	Detailed chemical kinetic modeling of JPâ€10 (exoâ€tetrahydrodicyclopentadiene) highâ€temperature oxidation: Exploring the role of biradical species in initial decomposition steps. International Journal of Chemical Kinetics, 2012, 44, 179-193.	1.6	43
101	Benchmarking the completely renormalised equation-of-motion coupled-cluster approaches for vertical excitation energies. Molecular Physics, 2015, 113, 3085-3127.	1.7	43
102	The state-universal multi-reference coupled-cluster theory with perturbative description of coreâ€“virtual excitations. Chemical Physics Letters, 2001, 334, 89-98.	2.6	41
103	The Electronic Structure and Vibrational Spectrum oftrans-HNOOâ€. Journal of Physical Chemistry A, 2004, 108, 2893-2903.	2.5	41
104	Coupled quasidiabatic potential energy surfaces for LiFH. Journal of Chemical Physics, 2002, 116, 8353.	3.0	40
105	Is the Mechanism of the [2+2] Cycloaddition of Cyclopentyne to Ethylene Concerted or Biradical? A Completely Renormalized Coupled Cluster Studyâ€. Journal of Physical Chemistry A, 2006, 110, 367-378.	2.5	40
106	On the solution of coupled-cluster equations in the fully correlated limit of cyclic polyene model. International Journal of Quantum Chemistry, 1991, 40, 9-34.	2.0	39
107	Property Evaluation Using the Two-Reference State-Universal Coupled-Cluster Method. The Journal of Physical Chemistry, 1995, 99, 15354-15368.	2.9	39
108	Complete set of solutions of the generalized Bloch equation. International Journal of Quantum Chemistry, 2000, 80, 757-781.	2.0	38

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109	Dynamics of harpooning studied by transition state spectroscopy NaÂ·Â·Â·FH. Faraday Discussions, 1997, 108, 411-425.	3.2	37
110	Method of moments for the continuous transition between the Brillouinâ€“Wigner-type and Rayleighâ€“SchrÃ¶dinger-type multireference coupled cluster theories. Molecular Physics, 2009, 107, 1209-1221.	1.7	35
111	Combining active-space coupled-cluster approaches with moment energy corrections via the CC(P;Q) methodology: connected quadruple excitations. Molecular Physics, 2017, 115, 2860-2891.	1.7	35
112	Stateâ€selective multiâ€reference coupledâ€cluster theory employing the singleâ€reference formalism: Application to an excited state of H8. Journal of Chemical Physics, 1995, 102, 3301-3306.	3.0	34
113	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.	3.0	34
114	Application of renormalized coupled-cluster methods to potential function of water. Theoretical Chemistry Accounts, 2008, 120, 59-78.	1.4	32
115	Geometries, Binding Energies, Ionization Potentials, and Electron Affinities of Metal Clusters: Mg_n^{0,ÂÂ±Â1}, n = 1â€“7. Journal of Physical Chemistry C, 2016, 120, 13275-13286.	3.1	32
116	New Alternatives for Electronic Structure Calculations: Renormalized, Extended, and Generalized Coupled-Cluster Theories. Progress in Theoretical Chemistry and Physics, 2003, , 119-206.	0.2	32
117	Extrapolating potential energy surfaces by scaling electron correlation at a single geometry. Chemical Physics Letters, 2006, 430, 448-453.	2.6	31
118	Coupled-Cluster and Configuration-Interaction Calculations for Heavy Nuclei. Physical Review Letters, 2007, 98, 112501.	7.8	30
119	Dynamics of harpooning studied by transition state spectroscopy. II. Liâ‹…â‹…FH. Journal of Chemical Physics, 2000, 113, 9897-9900.	3.0	29
120	Method of moments of coupled-cluster equations: The quasivariational and quadratic approximations. Journal of Chemical Physics, 2003, 119, 2951-2962.	3.0	29
121	Renormalized Coupled-Cluster Calculations of Reactive Potential Energy Surfaces:Â The BeFH Systemâ€. Journal of Physical Chemistry A, 2004, 108, 8878-8893.	2.5	29
122	Parallelization of multi-reference coupled-cluster method. Parallel Computing, 2000, 26, 913-943.	2.1	28
123	Extension of the active-space equation-of-motion coupled-cluster methods to radical systems: The EA-EOMCCSDt and IP-EOMCCSDt approaches. International Journal of Quantum Chemistry, 2006, 106, 2854-2874.	2.0	28
124	Breaking Bonds of Open-Shell Species with the Restricted Open-Shell Size Extensive Left Eigenstate Completely Renormalized Coupled-Cluster Method. Journal of Physical Chemistry A, 2008, 112, 11873-11884.	2.5	28
125	Accurate excited-state energetics by a combination of Monte Carlo sampling and equation-of-motion coupled-cluster computations. Journal of Chemical Physics, 2019, 150, 111101.	3.0	28
126	Spherical tensor theory of long-range interactions in a system ofNarbitrary molecules including quantum-mechanical many-body effects. Molecular Physics, 1986, 59, 1067-1083.	1.7	27

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127	Method of Moments of Coupled-Cluster Equations: Externally Corrected Approaches Employing Configuration Interaction Wave Functions. International Journal of Molecular Sciences, 2002, 3, 475-497.	4.1	27
128	Application of the CC(P;Q) Hierarchy of Coupled-Cluster Methods to the Beryllium Dimer. Journal of Physical Chemistry A, 2018, 122, 1350-1368.	2.5	27
129	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
130	On the significance of quadruply excited clusters in coupled-cluster calculations for the low-lying states of BN and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si70.gif" display="inline" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mtext>C</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:m Chemical Physics Letters, 2008, 461, 321-326.	2.6	26
131	Incorporating a completely renormalized coupled cluster approach into a composite method for thermodynamic properties and reaction paths. Journal of Chemical Physics, 2012, 136, 144109.	3.0	26
132	Communication: Determining the lowest-energy isomer of Au8: 2D, or not 2D. Journal of Chemical Physics, 2013, 139, 091101.	3.0	26
133	Spherical tensor theory of long-range interactions in a system ofNarbitrary molecules including quantum-mechanical many-body effects. Molecular Physics, 1986, 59, 1085-1095.	1.7	25
134	Non-iterative coupled-cluster methods employing multi-reference perturbation theory wave functions. Computational and Theoretical Chemistry, 2006, 771, 89-104.	1.5	24
135	Bound and quasibound states of the Naâ‹¯FH van der Waals molecule. Journal of Chemical Physics, 2000, 112, 189-202.	3.0	23
136	Behavior of coupled cluster energy in the strongly correlated limit of the cyclic polyene model. Comparison with the exact results. International Journal of Quantum Chemistry, 1992, 42, 165-191.	2.0	22
137	Potential energy curves for the HFâ¯ and CH3Fâ¯ anions: a coupled cluster study. Journal of Molecular Structure, 1997, 436-437, 503-536.	3.6	22
138	Extrapolating potential energy surfaces by scaling electron correlation: Isomerization of bicyclobutane to butadiene. Journal of Chemical Physics, 2008, 128, 154116.	3.0	22
139	Doubly electron-attached and doubly ionised equation-of-motion coupled-cluster methods withÂfull and active-space treatments of 4-particleâ€“2-hole and 4-holeâ€“2-particle excitations: the role ofÂorbital choices. Molecular Physics, 2014, 112, 868-885.	1.7	21
140	Molecular quadrupole moment functions of HF and N2. II. Rovibrational effects. Journal of Chemical Physics, 1996, 104, 4716-4727.	3.0	20
141	A comparative assessment of the perturbative and renormalized coupled cluster theories with a noniterative treatment of triple excitations for thermochemical kinetics, including a study of basis set and core correlation effects. Journal of Chemical Physics, 2008, 128, 044108.	3.0	20
142	Systematic design of active spaces for multi-reference calculations of singletâ€“triplet gaps of organic diradicals, with benchmarks against doubly electron-attached coupled-cluster data. Journal of Chemical Physics, 2017, 147, 164120.	3.0	20
143	Spherical tensor theory of long-range interactions between two molecules. International Journal of Quantum Chemistry, 1984, 25, 449-473.	2.0	19
144	Theoretical studies of lithium bonding in lithium chloride/aliphatic amine complexes. Chemical Physics, 1985, 94, 55-63.	1.9	18

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145	Coupled-cluster approaches with an approximate account of triexcitations and the optimized-inner-projection technique. III. Lower bounds to the ground-state correlation energy of cyclic-polyene model systems. Physical Review A, 1990, 42, 5155-5167.	2.5	18
146	Molecular quadrupole moment function of ammonia. Journal of Chemical Physics, 1996, 105, 11068-11074.	3.0	18
147	A General Reaction Path Dual-Level Direct Dynamics Calculation of the Reaction of Hydroxyl Radical with Dimethyl Sulfide. Journal of Physical Chemistry A, 2000, 104, 8779-8786.	2.5	18
148	Diffusion of Atomic Oxygen on the Si(100) Surface. Journal of Physical Chemistry C, 2010, 114, 12649-12658.	3.1	18
149	Aerobic Oxidation of Methanol to Formic Acid on Au₈^{â€“}: Benchmark Analysis Based on Completely Renormalized Coupled-Cluster and Density Functional Theory Calculations. Journal of Physical Chemistry A, 2013, 117, 10416-10427.	2.5	18
150	Can a Single-Reference Approach Provide a Balanced Description of Ground and Excited States? A Comparison of the Completely Renormalized Equation-of-Motion Coupled-Cluster Method with Multireference Quasidegenerate Perturbation Theory near a Conical Intersection and along a Photodissociation Coordinate in Ammonia. Journal of Physical Chemistry A, 2005, 109, 11643-11646.	2.5	17
151	Nuclear Structure Calculations with Coupled Cluster Methods from Quantum Chemistry. Nuclear Physics A, 2005, 752, 299-308.	1.5	16
152	Intricacies of van der Waals Interactions in Systems with Elongated Bonds Revealed by Electron-Groups Embedding and High-Level Coupled-Cluster Approaches. Journal of Chemical Theory and Computation, 2017, 13, 5404-5419.	5.3	16
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