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	Addressing strong correlation by approximate coupled-pair methods with active-space and full treatments of three-body clusters. Molecular Physics, 2022, 120, .	1.7	5
2	High-level coupled-cluster energetics by Monte Carlo sampling and moment expansions: Further details and comparisons. Journal of Chemical Physics, 2021, 154, 124103.	3.0	12
3	Is Externally Corrected Coupled Cluster Always Better Than the Underlying Truncated Configuration Interaction?. Journal of Chemical Theory and Computation, 2021, 17, 4006-4027.	5.3	14
4	Controlling Quantum Interference between Virtual and Dipole Two-Photon Optical Excitation Pathways Using Phase-Shaped Laser Pulses. Journal of Physical Chemistry A, 2021, 125, 7534-7544.	2.5	8
5	Double electron-attachment equation-of-motion coupled-cluster methods with up to 4-particleâ€“2-hole excitations: improved implementation and application to singletâ€“triplet gaps in ortho- , meta- , and para- benzyne isomers. Molecular Physics, 2021, 119, .	1.7	7
6	Internal Conversion between Bright (1¹B_u⁺) and Dark (2¹A_g^{â€“}) States in s-trans-Butadiene and s-trans-Hexatriene. Journal of Physical Chemistry Letters, 2021, 12, 9720-9729.	4.6	14
7	High-level coupled-cluster energetics by merging moment expansions with selected configuration interaction. Journal of Chemical Physics, 2021, 155, 174114.	3.0	10
8	Excited-State Dynamics of a Substituted Fluorene Derivative. The Central Role of Hydrogen Bonding Interactions with the Solvent. Journal of Physical Chemistry B, 2021, 125, 12242-12253.	2.6	2
9	Intramolecular Relaxation Dynamics Mediated by Solventâ€“Solute Interactions of Substituted Fluorene Derivatives. Solute Structural Dependence. Journal of Physical Chemistry B, 2021, 125, 12486-12499.	2.6	0
10	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
11	The Ground State Electronic Energy of Benzene. Journal of Physical Chemistry Letters, 2020, 11, 8922-8929.	4.6	90
12	Optimization of the Reax force field for the lithiumâ€“oxygen system using a high fidelity charge model. Journal of Chemical Physics, 2020, 153, 084107.	3.0	11
13	Steric effects in light-induced solvent proton abstraction. Physical Chemistry Chemical Physics, 2020, 22, 19613-19622.	2.8	4
14	Accelerating convergence of equation-of-motion coupled-cluster computations using the semi-stochastic CC(P;Q) formalism. Molecular Physics, 2020, 118, e1817592.	1.7	11
15	Quantum computation solves a half-century-old enigma: Elusive vibrational states of magnesium dimer found. Science Advances, 2020, 6, eaay4058.	10.3	15
16	Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102.	3.0	734
17	Isoenergetic two-photon excitation enhances solvent-to-solute excited-state proton transfer. Journal of Chemical Physics, 2020, 153, 224301.	3.0	4
18	Proton Abstraction Mediates Interactions between the Super Photobase FR0-SB and Surrounding Alcohol Solvent. Journal of Physical Chemistry B, 2019, 123, 8448-8456.	2.6	9

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19	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
20	Application of the coupled-cluster CC(P;Q) approaches to the magnesium dimer. Molecular Physics, 2019, 117, 1486-1506.	1.7	11
21	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
22	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
23	Femtosecond real-time probing of reactions MMXVII: The predissociation of sodium iodide in the A 0+ state. Chemical Physics Letters, 2017, 683, 121-127.	2.6	6
24	Economical Doubly Electron-Attached Equation-of-Motion Coupled-Cluster Methods with an Active-Space Treatment of Three-Particleâ€“One-Hole and Four-Particleâ€“Two-Hole Excitations. Journal of Physical Chemistry A, 2017, 121, 3469-3485.	2.5	14
25	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
26	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
27	Converging High-Level Coupled-Cluster Energetics by MonteÂCarlo Sampling and Moment Expansions. Physical Review Letters, 2017, 119, 223003.	7.8	73
28	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
29	Coupled-cluster interpretation of the photoelectron spectrum of Ag3â¯. Journal of Chemical Physics, 2016, 145, 084306.	3.0	3
30	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
31	Ab initiocoupled-cluster and multi-reference configuration interaction studies of the low-lying electronic states of 1,2,3,4-cyclobutanetetraone. Molecular Physics, 2016, 114, 695-708.	1.7	3
32	Dealing with chemical reaction pathways and electronic excitations in molecular systems via renormalized and active-space coupled-cluster methods. , 2015, , .		0
33	Benchmarking the completely renormalised equation-of-motion coupled-cluster approaches for vertical excitation energies. Molecular Physics, 2015, 113, 3085-3127.	1.7	43
34	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
35	Communication: Coupled-cluster interpretation of the photoelectron spectrum of ${m Au}_{3}^{-}$ Au 3â¯. Journal of Chemical Physics, 2014, 141, 101102.	3.0	6
36	Performance of the completely renormalized equation-of-motion coupled-cluster method in calculations of excited-state potential cuts of water. Computational and Theoretical Chemistry, 2014, 1040-1041, 20-34.	2.5	10

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37	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
38	Evaluation of density functional methods on the geometric and energetic descriptions of species involved in Cu+-promoted catalysis. Journal of Molecular Modeling, 2013, 19, 5457-5467.	1.8	8
39	Communication: Determining the lowest-energy isomer of Au8: 2D, or not 2D. Journal of Chemical Physics, 2013, 139, 091101.	3.0	26
40	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
41	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
42	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
43	Communication: Existence of the doubly excited state that mediates the photoionization of azulene. Journal of Chemical Physics, 2013, 138, 201102.	3.0	14
44	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
45	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
46	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
47	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
48	Quantum Systems in Chemistry and Physics. Progress in Theoretical Chemistry and Physics, 2012, , .	0.2	6
49	Shifts in Excitation Energies Induced by Hydrogen Bonding: A Comparison of the Embedding and Supermolecular Time-Dependent Density Functional Theory Calculations with the Equation-of-Motion Coupled-Cluster Results. Progress in Theoretical Chemistry and Physics, 2012, , 219-248.	0.2	7
50	Symmetry-adapted-cluster configuration-interaction and equation-of-motion coupled-cluster studies of electronically excited states of copper tetrachloride and copper tetrabromide dianions. Chemical Physics, 2012, 399, 94-110.	1.9	8
51	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
52	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
53	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
54	Geometries and adiabatic excitation energies of the low-lying valence states of CNC, C₂N, N₃and NCO studied with the electron-attached and ionized equation-of-motion coupled-cluster methodologies. Physica Scripta, 2011, 84, 028110.	2.5	9

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55	Diffusion of Atomic Oxygen on the Si(100) Surface. Journal of Physical Chemistry C, 2010, 114, 12649-12658.	3.1	18
56	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
57	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
58	Comparison of the completely renormalized equation-of-motion coupled-cluster and Quantum Monte Carlo results for the low-lying electronic states of methylene. Molecular Physics, 2010, 108, 2633-2646.	1.7	13
59	Active-space coupled-cluster methods. Molecular Physics, 2010, 108, 2987-3015.	1.7	80
60	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
61	Local Correlation Calculations Using Standard and Renormalized Coupled-Cluster Methods. , 2009, , .		9
62	Local correlation calculations using standard and renormalized coupled-cluster approaches. Journal of Chemical Physics, 2009, 131, 114109.	3.0	199
63	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
64	Center-of-mass problem in truncated configuration interaction and coupled-cluster calculations. Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics, 2009, 679, 334-339.	4.1	13
65	Advances in the Theory of Atomic and Molecular Systems. Progress in Theoretical Chemistry and Physics, 2009, , .	0.2	3
66	Thermochemical Kinetics for Multireference Systems: Addition Reactions of Ozone. Journal of Physical Chemistry A, 2009, 113, 5786-5799.	2.5	114
67	Ab initio coupled-cluster and configuration interaction calculations for <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mmultiscripts><mml:mi mathvariant="normal">O</mml:mi><mml:mprescripts /><mml:none /><mml:mrow><mml:mn>16</mml:mn></mml:mrow></mml:mmultiscripts></mml:math> using the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>V</mml:mi><mml:mrow><mml:mi mathvariant="normal	2.9	13
68	Advances in the Theory of Atomic and Molecular Systems. Progress in Theoretical Chemistry and Physics, 2009, , .	0.2	9
69	Low-lying valence excited states of CNC, C₂N, N₃, and NCO studied using the electron-attached and ionized symmetry-adapted-cluster configuration-interaction and equation-of-motion coupled-cluster methodologies. Molecular Physics, 2009, 107, 871-880.	1.7	15
70	Linear Scaling Local Correlation Extensions of the Standard and Renormalized Coupled-Cluster Methods. Progress in Theoretical Chemistry and Physics, 2009, , 131-195.	0.2	5
71	Application of renormalized coupled-cluster methods to potential function of water. Theoretical Chemistry Accounts, 2008, 120, 59-78.	1.4	32
72	Biorthogonal method of moments of coupledâ€cluster equations: Alternative derivation, further considerations, and application to a model magnetic system. International Journal of Quantum Chemistry, 2008, 108, 2128-2149.	2.0	14

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73	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:mn> Chemical Physics Letters, 2008, 461, 321-326.	2.6	26
74	A comparison of single-reference coupled-cluster and multi-reference configuration interaction methods for representative cuts of the potential energy surface. Computational and Theoretical Chemistry, 2008, 859, 22-29.	1.5	14
75	Frontiers in Quantum Systems in Chemistry and Physics. Progress in Theoretical Chemistry and Physics, 2008, , .	0.2	14
76	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
77	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
78	Extrapolating potential energy surfaces by scaling electron correlation: Isomerization of bicyclobutane to butadiene. Journal of Chemical Physics, 2008, 128, 154116.	3.0	22
79	Nondynamic Correlation and Coupled-Cluster Methods. AIP Conference Proceedings, 2008, , .	0.4	0
80	Extrapolating Potential Energy Surfaces by Scaling Electron Correlation: Isomerization of Bicyclobutane to Butadiene. AIP Conference Proceedings, 2008, , .	0.4	1
81	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
82	Coupled-Cluster and Configuration-Interaction Calculations for Odd-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>A</mml:mi></mml:math>Heavy Nuclei. Physical Review Letters, 2008, 101, 052501.	7.8	12
83	Front Matter for Volume 995. AIP Conference Proceedings, 2008, , .	0.4	0
84	Method of Moments of Coupled Cluster Equations Employing Multi-Reference Perturbation Theory Wavefunctions: General Formalism, Diagrammatic Formulation, Implementation, and Benchmark Studies. Progress in Theoretical Chemistry and Physics, 2008, , 67-174.	0.2	1
85	Coupled-Cluster and Configuration-Interaction Calculations for Heavy Nuclei. Physical Review Letters, 2007, 98, 112501.	7.8	30
86	Coupled-cluster theory for three-body Hamiltonians. Physical Review C, 2007, 76, .	2.9	147
87	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
88	Breaking bonds with the left eigenstate completely renormalized coupled-cluster method. Journal of Chemical Physics, 2007, 127, 174106.	3.0	63
89	New Alternatives for Accurate Electronic Structure Calculations of Potential Energy Surfaces Involving Bond Breaking. ACS Symposium Series, 2007, , 37-73.	0.5	7
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	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
92	Renormalized coupled-cluster methods: Theoretical foundations and application to the potential function of water. Progress in Theoretical Chemistry and Physics, 2007, , 63-121.	0.2	16
93	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
94	Experimental and Theoretical UV Characterizations of Acetylacetone and Its Isomers. Journal of Physical Chemistry A, 2006, 110, 3920-3926.	2.5	51
95	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
96	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
97	COUPLED-CLUSTER THEORY FOR NUCLEI. , 2006, , .		0
98	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
99	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
100	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
101	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
102	Single-reference, size-extensive, non-iterative coupled-cluster approaches to bond breaking and biradicals. Chemical Physics Letters, 2006, 418, 467-474.	2.6	180
103	Extrapolating potential energy surfaces by scaling electron correlation at a single geometry. Chemical Physics Letters, 2006, 430, 448-453.	2.6	31
104	Non-iterative coupled-cluster methods employing multi-reference perturbation theory wave functions. Computational and Theoretical Chemistry, 2006, 771, 89-104.	1.5	24
105	Intriguing accuracies of the exponential wave function expansions exploiting finite two-body correlation operators in calculations for many-electron systems. Computational and Theoretical Chemistry, 2006, 768, 3-16.	1.5	6
106	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
107	Coupled-cluster calculations for valence systems aroundO16. Physical Review C, 2006, 74, .	2.9	64
108	NONITERATIVE COUPLED-CLUSTER METHODS FOR EXCITED ELECTRONIC STATES. , 2006, , 45-106.		7

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109	COUPLED-CLUSTER THEORY FOR NUCLEI. International Journal of Modern Physics B, 2006, 20, 5338-5345.	2.0	4
110	COUPLED CLUSTER APPROACHES TO NUCLEI, GROUND STATES AND EXCITED STATES. , 2005, , .		0
111	Nuclear Structure Calculations with Coupled Cluster Methods from Quantum Chemistry. Nuclear Physics A, 2005, 752, 299-308.	1.5	16
112	Ab initio coupled cluster calculations for nuclei using methods of quantum chemistry. European Physical Journal A, 2005, 25, 485-488.	2.5	3
113	Where Does the Planar-to-Nonplanar Turnover Occur in Small Gold Clusters?. ChemInform, 2005, 36, no.	0.0	0
114	Bridging quantum chemistry and nuclear structure theory: Coupled-cluster calculations for closed- and open-shell nuclei. AIP Conference Proceedings, 2005, , .	0.4	3
115	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
116	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
117	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
118	Comparison of low-order multireference many-body perturbation theories. Journal of Chemical Physics, 2005, 122, 134105.	3.0	62
119	Coupled-cluster calculations for ground and excited states of closed- and open-shell nuclei using methods of quantum chemistry. Journal of Physics G: Nuclear and Particle Physics, 2005, 31, S1291-S1299.	3.6	8
120	Renormalized coupled-cluster methods exploiting left eigenstates of the similarity-transformed Hamiltonian. Journal of Chemical Physics, 2005, 123, 224105.	3.0	391
121	Active-space coupled-cluster study of electronic states of Be3. Journal of Chemical Physics, 2005, 123, 074319.	3.0	59
122	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
123	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
124	Ab-InitioCoupled-Cluster Study ofO16. Physical Review Letters, 2005, 94, 212501.	7.8	100
125	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
126	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

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127	Extensive generalization of renormalized coupled-cluster methods. Journal of Chemical Physics, 2005, 122, 074107.	3.0	96
128	Ab initio coupled cluster calculations for nuclei using methods of quantum chemistry. , 2005, , 485-488.		0
129	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
130	New classes of non-iterative energy corrections to multi-reference coupled-cluster energies. Molecular Physics, 2004, 102, 2425-2449.	1.7	58
131	The Electronic Structure and Vibrational Spectrum oftrans-HNOOâ€. Journal of Physical Chemistry A, 2004, 108, 2893-2903.	2.5	41
132	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
133	Combined coupled-cluster and many-body perturbation theories. Journal of Chemical Physics, 2004, 121, 12197.	3.0	161
134	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
135	Coupled Cluster Calculations of Ground and Excited States of Nuclei. Physical Review Letters, 2004, 92, 132501.	7.8	119
136	Exactness of Two-Body Cluster Expansions in Many-Body Quantum Theory. Physical Review Letters, 2003, 90, 113001.	7.8	43
137	Method of moments of coupled-cluster equations: The quasivariational and quadratic approximations. Journal of Chemical Physics, 2003, 119, 2951-2962.	3.0	29
138	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
139	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
140	Coupled quasidiabatic potential energy surfaces for LiFH. Journal of Chemical Physics, 2002, 116, 8353.	3.0	40
141	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
142	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
143	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
144	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

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145	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
146	Bound and quasi-bound states of the Liâ‹¯FH van der Waals molecule: The effects of the potential energy surface and of the basis set superposition error. Computational and Theoretical Chemistry, 2002, 591, 151-174.	1.5	10
147	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
148	Can NO2+ exist in bent or cyclic forms?. Chemical Physics Letters, 2001, 334, 381-386.	2.6	3
149	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
150	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
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