Piotr Piecuch

List of Publications by Year in Descending Order

225 papers	11,913 citations	59 h-index	100 g-index
241 ext. papers	12,601 ext. citations	3.2 avg, IF	6.47 L-index

#	Paper	IF	Citations
225	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	3.4	2
224	Intramolecular Relaxation Dynamics Mediated by Solvent-Solute Interactions of Substituted Fluorene Derivatives. Solute Structural Dependence. *Journal of Physical Chemistry B*, **2021**, 125, 12486-12499	3.4	
223	High-level coupled-cluster energetics by merging moment expansions with selected configuration interaction. *Journal of Chemical Physics*, **2021**, 155, 174114	3.9	2
222	High-level coupled-cluster energetics by Monte Carlo sampling and moment expansions: Further details and comparisons. *Journal of Chemical Physics*, **2021**, 154, 124103	3.9	6
221	Is Externally Corrected Coupled Cluster Always Better Than the Underlying Truncated Configuration Interaction?. *Journal of Chemical Theory and Computation*, **2021**, 17, 4006-4027	6.4	7
220	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	2.8	2
219	Internal Conversion between Bright (1) and Dark (2) States in s--Butadiene and s--Hexatriene. *Journal of Physical Chemistry Letters*, **2021**, 12, 9720-9729	6.4	4
218	Quantum computation solves a half-century-old enigma: Elusive vibrational states of magnesium dimer found. *Science Advances*, **2020**, 6, eaay4058	14.3	5
217	Isoenergetic two-photon excitation enhances solvent-to-solute excited-state proton transfer. *Journal of Chemical Physics*, **2020**, 153, 224301	3.9	3
216	Photoluminescence, photophysics, and photochemistry of the VB□ defect in hexagonal boron nitride. *Physical Review B*, **2020**, 102,	3.3	21
215	The Ground State Electronic Energy of Benzene. *Journal of Physical Chemistry Letters*, **2020**, 11, 8922-8929	6.4	52
214	Optimization of the Reax force field for the lithium-oxygen system using a high fidelity charge model. *Journal of Chemical Physics*, **2020**, 153, 084107	3.9	5
213	Steric effects in light-induced solvent proton abstraction. *Physical Chemistry Chemical Physics*, **2020**, 22, 19613-19622	3.6	4
212	Accelerating convergence of equation-of-motion coupled-cluster computations using the semi-stochastic CC(P;Q) formalism. *Molecular Physics*, **2020**, 118, e1817592	1.7	9
211	Recent developments in the general atomic and molecular electronic structure system. *Journal of Chemical Physics*, **2020**, 152, 154102	3.9	274
210	Proton Abstraction Mediates Interactions between the Super Photobase FR0-SB and Surrounding Alcohol Solvent. *Journal of Physical Chemistry B*, **2019**, 123, 8448-8456	3.4	8
209	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	3.9	24

208	Application of the coupled-cluster CC(P;Q) approaches to the magnesium dimer. *Molecular Physics*, **2019**, 117, 1486-1506	1.7	7
207	Application of the CC(P;Q) Hierarchy of Coupled-Cluster Methods to the Beryllium Dimer. *Journal of Physical Chemistry A*, **2018**, 122, 1350-1368	2.8	25
206	Communication: Approaching exact quantum chemistry by cluster analysis of full configuration interaction quantum Monte Carlo wave functions. *Journal of Chemical Physics*, **2018**, 149, 151101	3.9	47
205	Femtosecond real-time probing of reactions MMXVII: The predissociation of sodium iodide in the A 0+ state. *Chemical Physics Letters*, **2017**, 683, 121-127	2.5	4
204	Economical Doubly Electron-Attached Equation-of-Motion Coupled-Cluster Methods with an Active-Space Treatment of Three-Particle-One-Hole and Four-Particle-Two-Hole Excitations. *Journal of Physical Chemistry A*, **2017**, 121, 3469-3485	2.8	12
203	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	6.4	12
202	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	27
201	Converging High-Level Coupled-Cluster Energetics by Monte□Carlo Sampling and Moment Expansions. *Physical Review Letters*, **2017**, 119, 223003	7.4	56
200	Systematic design of active spaces for multi-reference calculations of singlet-triplet gaps of organic diradicals, with benchmarks against doubly electron-attached coupled-cluster data. *Journal of Chemical Physics*, **2017**, 147, 164120	3.9	18
199	Coupled-cluster interpretation of the photoelectron spectrum of Ag3 (.). *Journal of Chemical Physics*, **2016**, 145, 084306	3.9	3
198	Geometries, Binding Energies, Ionization Potentials, and Electron Affinities of Metal Clusters: Mgn0, □ 1, n = 1□. *Journal of Physical Chemistry C*, **2016**, 120, 13275-13286	3.8	27
197	Ab initio coupled-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	2
196	Benchmarking the completely renormalised equation-of-motion coupled-cluster approaches for vertical excitation energies. *Molecular Physics*, **2015**, 113, 3085-3127	1.7	32
195	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	8
194	Doubly electron-attached and doubly ionised equation-of-motion coupled-cluster methods with full and active-space treatments of 4-particle□-hole and 4-hole□-particle excitations: the role of orbital choices. *Molecular Physics*, **2014**, 112, 868-885	1.7	19
193	Communication: Coupled-cluster interpretation of the photoelectron spectrum of Au□. *Journal of Chemical Physics*, **2014**, 141, 101102	3.9	6
192	Aerobic oxidation of methanol to formic acid on Au8-: benchmark analysis based on completely renormalized coupled-cluster and density functional theory calculations. *Journal of Physical Chemistry A*, **2013**, 117, 10416-27	2.8	17
191	Evaluation of density functional methods on the geometric and energetic descriptions of species involved in Cu+-promoted catalysis. *Journal of Molecular Modeling*, **2013**, 19, 5457-67	2	6

190	Communication: Determining the lowest-energy isomer of Au8: 2D, or not 2D. *Journal of Chemical Physics*, **2013**, 139, 091101	3.9	22
189	Electronic structure of the S1 state in methylcobalamin: insight from CASSCF/MC-XQDPT2, EOM-CCSD, and TD-DFT calculations. *Journal of Computational Chemistry*, **2013**, 34, 987-1004	3.5	49
188	Doubly electron-attached and doubly ionized equation-of-motion coupled-cluster methods with 4-particle-2-hole and 4-hole-2-particle excitations and their active-space extensions. *Journal of Chemical Physics*, **2013**, 138, 194102	3.9	63
187	Extension of coupled-cluster theory with a noniterative treatment of connected triply excited clusters to three-body Hamiltonians. *Physical Review C*, **2013**, 88,	2.7	51
186	Communication: existence of the doubly excited state that mediates the photoionization of azulene. *Journal of Chemical Physics*, **2013**, 138, 201102	3.9	13
185	Detailed chemical kinetic modeling of JP-10 (exo-tetrahydrodicyclopentadiene) high-temperature oxidation: Exploring the role of biradical species in initial decomposition steps. *International Journal of Chemical Kinetics*, **2012**, 44, 179-193	1.4	38
184	Merging Active-Space and Renormalized Coupled-Cluster Methods via the CC(P;Q) Formalism, with Benchmark Calculations for Singlet-Triplet Gaps in Biradical Systems. *Journal of Chemical Theory and Computation*, **2012**, 8, 4968-88	6.4	44
183	Incorporating a completely renormalized coupled cluster approach into a composite method for thermodynamic properties and reaction paths. *Journal of Chemical Physics*, **2012**, 136, 144109	3.9	22
182	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	3.9	49
181	The Cobalt-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, 1870-94	6.4	78
180	Quantum Systems in Chemistry and Physics. *Progress in Theoretical Chemistry and Physics*, **2012**,	0.6	2
179	Advances in the Theory of Quantum Systems in Chemistry and Physics. *Progress in Theoretical Chemistry and Physics*, **2012**,	0.6	3
178	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	0.6	7
177	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	2.3	7
176	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	2.3	61
175	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	2.6	9
174	Embedding vs Supermolecular Strategies in Evaluating the Hydrogen-Bonding-Induced Shifts of Excitation Energies. *Journal of Chemical Theory and Computation*, **2011**, 7, 1647-1666	6.4	56
173	Diffusion of Atomic Oxygen on the Si(100) Surface. *Journal of Physical Chemistry C*, **2010**, 114, 12649-12658	3.8	15

172	Multilevel extension of the cluster-in-molecule local correlation methodology: merging coupled-cluster and Møller-Plesset perturbation theories. *Journal of Physical Chemistry A*, **2010**, 114, 6721-7	2.8	92
171	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. *Journal of Physical Chemistry A*, **2010**, 114, 8644-57	2.8	79
170	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
169	Active-space coupled-cluster methods. *Molecular Physics*, **2010**, 108, 2987-3015	1.7	68
168	Method of moments for the continuous transition between the Brillouin–Wigner-type and Rayleigh–Schrödinger-type multireference coupled cluster theories. *Molecular Physics*, **2009**, 107, 1209-1221	1.7	34
167	Local Correlation Calculations Using Standard and Renormalized Coupled-Cluster Methods **2009**,		9
166	Local correlation calculations using standard and renormalized coupled-cluster approaches. *Journal of Chemical Physics*, **2009**, 131, 114109	3.9	177
165	Left-eigenstate completely renormalized equation-of-motion coupled-cluster methods: Review of key concepts, extension to excited states of open-shell systems, and comparison with electron-attached and ionized approaches. *International Journal of Quantum Chemistry*, **2009**, 109, 3268-3304	2.1	97
164	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	4.2	10
163	Advances in the Theory of Atomic and Molecular Systems. *Progress in Theoretical Chemistry and Physics*, **2009**,	0.6	3
162	Thermochemical kinetics for multireference systems: addition reactions of ozone. *Journal of Physical Chemistry A*, **2009**, 113, 5786-99	2.8	106
161	Ab initio coupled-cluster and configuration interaction calculations for O16 using the VUCOM interaction. *Physical Review C*, **2009**, 79,	2.7	12
160	Advances in the Theory of Atomic and Molecular Systems. *Progress in Theoretical Chemistry and Physics*, **2009**,	0.6	6
159	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
158	Linear Scaling Local Correlation Extensions of the Standard and Renormalized Coupled-Cluster Methods. *Progress in Theoretical Chemistry and Physics*, **2009**, 131-195	0.6	4
157	Frontiers in Quantum Systems in Chemistry and Physics. *Progress in Theoretical Chemistry and Physics*, **2008**,	0.6	5
156	Stereoelectronic effects on molecular geometries and state-energy splittings of ligated monocopper dioxygen complexes. *Journal of Physical Chemistry A*, **2008**, 112, 3754-67	2.8	56
155	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, 11873-84	2.8	27

154	Extrapolating potential energy surfaces by scaling electron correlation: isomerization of bicyclobutane to butadiene. *Journal of Chemical Physics*, **2008**, 128, 154116	3.9	21
153	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	3.9	20
152	Coupled-cluster and configuration-interaction calculations for odd-A heavy nuclei. *Physical Review Letters*, **2008**, 101, 052501	7.4	11
151	Application of renormalized coupled-cluster methods to potential function of water. *Theoretical Chemistry Accounts*, **2008**, 120, 59-78	1.9	30
150	Biorthogonal method of moments of coupled-cluster equations: Alternative derivation, further considerations, and application to a model magnetic system. *International Journal of Quantum Chemistry*, **2008**, 108, 2128-2149	2.1	11
149	On the significance of quadruply excited clusters in coupled-cluster calculations for the low-lying states of BN and C2. *Chemical Physics Letters*, **2008**, 461, 321-326	2.5	25
148	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		14
147	Extension of the renormalized coupled-cluster methods exploiting left eigenstates of the similarity-transformed hamiltonian to open-shell systems: a benchmark study. *Journal of Physical Chemistry A*, **2007**, 111, 11359-82	2.8	160
146	Coupled-cluster and configuration-interaction calculations for heavy nuclei. *Physical Review Letters*, **2007**, 98, 112501	7.4	27
145	Coupled-cluster theory for three-body Hamiltonians. *Physical Review C*, **2007**, 76,	2.7	129
144	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	3.9	44
143	Breaking bonds with the left eigenstate completely renormalized coupled-cluster method. *Journal of Chemical Physics*, **2007**, 127, 174106	3.9	59
142	New Alternatives for Accurate Electronic Structure Calculations of Potential Energy Surfaces Involving Bond Breaking. *ACS Symposium Series*, **2007**, 37-73	0.4	7
141	Computational investigation of the conrotatory and disrotatory isomerization channels of bicyclo[1.1.0]butane to buta-1,3-diene: a completely renormalized coupled-cluster study. *Journal of Physical Chemistry A*, **2007**, 111, 734-42	2.8	46
140	Renormalized coupled-cluster methods: Theoretical foundations and application to the potential function of water. *Progress in Theoretical Chemistry and Physics*, **2007**, 63-121	0.6	14
139	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	101
138	Coupled-cluster calculations for valence systems around O16. *Physical Review C*, **2006**, 74,	2.7	61
137	NONITERATIVE COUPLED-CLUSTER METHODS FOR EXCITED ELECTRONIC STATES **2006**, 45-106		5

136	COUPLED-CLUSTER THEORY FOR NUCLEI. *International Journal of Modern Physics B*, **2006**, 20, 5338-5345	1.1	4
135	Theoretical characterization of end-on and side-on peroxide coordination in ligated Cu2O2 models. *Journal of Physical Chemistry A*, **2006**, 110, 11557-68	2.8	72
134	Experimental and theoretical UV characterizations of acetylacetone and its isomers. *Journal of Physical Chemistry A*, **2006**, 110, 3920-6	2.8	50
133	Is the mechanism of the [2+2] cycloaddition of cyclopentyne to ethylene concerted or biradical? A completely renormalized coupled cluster study. *Journal of Physical Chemistry A*, **2006**, 110, 367-78	2.8	36
132	Theoretical models on the Cu2O2 torture track: mechanistic implications for oxytyrosinase and small-molecule analogues. *Journal of Physical Chemistry A*, **2006**, 110, 1991-2004	2.8	157
131	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	1.4	40
130	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	3.9	87
129	Automated derivation and parallel computer implementation of renormalized and active-space coupled-cluster methods. *International Journal of Quantum Chemistry*, **2006**, 106, 79-97	2.1	51
128	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	2.1	27
127	Single-reference, size-extensive, non-iterative coupled-cluster approaches to bond breaking and biradicals. *Chemical Physics Letters*, **2006**, 418, 467-474	2.5	171
126	Extrapolating potential energy surfaces by scaling electron correlation at a single geometry. *Chemical Physics Letters*, **2006**, 430, 448-453	2.5	31
125	Non-iterative coupled-cluster methods employing multi-reference perturbation theory wave functions. *Computational and Theoretical Chemistry*, **2006**, 771, 89-104		21
124	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		5
123	Renormalized coupled-cluster methods exploiting left eigenstates of the similarity-transformed Hamiltonian. *Journal of Chemical Physics*, **2005**, 123, 224105	3.9	364
122	Active-space coupled-cluster study of electronic states of Be3. *Journal of Chemical Physics*, **2005**, 123, 074319	3.9	58
121	Balancing dynamic and nondynamic correlation for diradical and aromatic transition states: a renormalized coupled-cluster study of the cope rearrangement of 1,5-hexadiene. *Journal of the American Chemical Society*, **2005**, 127, 2608-14	16.4	54
120	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	46
119	Ab-initio coupled-cluster study of 16O. *Physical Review Letters*, **2005**, 94, 212501	7.4	90

118	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, 11643-6	2.8	17
117	Where does the planar-to-nonplanar turnover occur in small gold clusters?. *Journal of the American Chemical Society*, **2005**, 127, 1049-52	16.4	198
116	Extensive generalization of renormalized coupled-cluster methods. *Journal of Chemical Physics*, **2005**, 122, 074107	3.9	94
115	Nuclear Structure Calculations with Coupled Cluster Methods from Quantum Chemistry. *Nuclear Physics A*, **2005**, 752, 299-308	1.3	16
114	Ab initio coupled cluster calculations for nuclei using methods of quantum chemistry. *European Physical Journal A*, **2005**, 25, 485-488	2.5	3
113	Bridging quantum chemistry and nuclear structure theory: Coupled-cluster calculations for closed- and open-shell nuclei. *AIP Conference Proceedings*, **2005**,	0	2
112	Extension of renormalized coupled-cluster methods including triple excitations to excited electronic states of open-shell molecules. *Journal of Chemical Physics*, **2005**, 122, 214107	3.9	109
111	The X1Sigmag+, B1Deltag, and BP1Sigmag+ states of C2: a comparison of renormalized coupled-cluster and multireference methods with full configuration interaction benchmarks. *Journal of Chemical Physics*, **2005**, 122, 124104	3.9	92
110	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	3.9	95
109	Comparison of low-order multireference many-body perturbation theories. *Journal of Chemical Physics*, **2005**, 122, 134105	3.9	58
108	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	2.9	8
107	Ab initio coupled cluster calculations for nuclei using methods of quantum chemistry **2005**, 485-488		
106	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	1.9	174
105	New classes of non-iterative energy corrections to multi-reference coupled-cluster energies. *Molecular Physics*, **2004**, 102, 2425-2449	1.7	54
104	The Electronic Structure and Vibrational Spectrum oftrans-HNOO *Journal of Physical Chemistry A*, **2004**, 108, 2893-2903	2.8	40
103	Renormalized Coupled-Cluster Calculations of Reactive Potential Energy Surfaces: The BeFH System *Journal of Physical Chemistry A*, **2004**, 108, 8878-8893	2.8	29
102	Combined coupled-cluster and many-body perturbation theories. *Journal of Chemical Physics*, **2004**, 121, 12197-207	3.9	156
101	New coupled-cluster methods with singles, doubles, and noniterative triples for high accuracy calculations of excited electronic states. *Journal of Chemical Physics*, **2004**, 120, 1715-38	3.9	282

100	Coupled cluster calculations of ground and excited states of nuclei. *Physical Review Letters*, **2004**, 92, 132501	7.4	109
99	Exactness of two-body cluster expansions in many-body quantum theory. *Physical Review Letters*, **2003**, 90, 113001	7.4	36
98	Method of moments of coupled-cluster equations: The quasivariational and quadratic approximations. *Journal of Chemical Physics*, **2003**, 119, 2951-2962	3.9	28
97	New Alternatives for Electronic Structure Calculations: Renormalized, Extended, and Generalized Coupled-Cluster Theories. *Progress in Theoretical Chemistry and Physics*, **2003**, 119-206	0.6	31
96	Method of Moments of Coupled-Cluster Equations: Externally Corrected Approaches Employing Configuration Interaction Wave Functions. *International Journal of Molecular Sciences*, **2002**, 3, 475-497	6.3	26
95	The State-Universal Multi-Reference Coupled-Cluster Theory: An Overview of Some Recent Advances. *International Journal of Molecular Sciences*, **2002**, 3, 676-709	6.3	49
94	Bound and quasi-bound states of the Li?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		10
93	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	4.2	420
92	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	3.9	34
91	Coupled quasidiabatic potential energy surfaces for LiFH. *Journal of Chemical Physics*, **2002**, 116, 8353	3.9	40
90	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	7	235
89	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	0.4	25
88	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	3.9	78
87	Can NO2+ exist in bent or cyclic forms?. *Chemical Physics Letters*, **2001**, 334, 381-386	2.5	3
86	The state-universal multi-reference coupled-cluster theory with perturbative description of core□virtual excitations. *Chemical Physics Letters*, **2001**, 334, 89-98	2.5	40
85	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	2.5	133
84	Excited-state potential energy curves of CH+: a comparison of the EOMCCSDt and full EOMCCSDT results. *Chemical Physics Letters*, **2001**, 347, 237-246	2.5	111
83	The active-space equation-of-motion coupled-cluster methods for excited electronic states: Full EOMCCSDt. *Journal of Chemical Physics*, **2001**, 115, 643-651	3.9	239

82	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	2.5	95
81	Extension of the method of moments of coupled-cluster equations to a multireference wave operator formalism. *Computational and Theoretical Chemistry*, **2001**, 547, 191-208		80
80	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	3.9	53
79	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	3.9	102
78	Photodissociation of LiFH and NaFH van der Waals complexes: A semiclassical trajectory study. *Journal of Chemical Physics*, **2001**, 115, 7945-7952	3.9	39
77	Complete set of solutions of the generalized Bloch equation. *International Journal of Quantum Chemistry*, **2000**, 80, 757-781	2.1	37
76	Bound and quasi-bound states of the Li?FH van der Waals molecule. *International Journal of Quantum Chemistry*, **2000**, 80, 916-933	2.1	13
75	Lifetimes and dissociation pathways of the quasi-bound states of the Na?FH van der Waals molecule. *Journal of Molecular Structure*, **2000**, 555, 43-60	3.4	5
74	Parallelization of multi-reference coupled-cluster method. *Parallel Computing*, **2000**, 26, 913-943	1	28
73	In Search of the Relationship between Multiple Solutions Characterizing Coupled-Cluster Theories. *Computational Chemistry - Reviews of Current Trends*, **2000**, 1-104		60
72	Complete set of solutions of multireference coupled-cluster equations: The state-universal formalism. *Physical Review A*, **2000**, 61,	2.6	82
71	Renormalized CCSD(T) and CCSD(TQ) approaches: Dissociation of the N2 triple bond. *Journal of Chemical Physics*, **2000**, 113, 5644-5652	3.9	193
70	Bound and quasibound states of the Na?FH van der Waals molecule. *Journal of Chemical Physics*, **2000**, 112, 189-202	3.9	19
69	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	2.8	17
68	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	3.9	361
67	The active-space equation-of-motion coupled-cluster methods for excited electronic states: The EOMCCSDt approach. *Journal of Chemical Physics*, **2000**, 113, 8490-8502	3.9	133
66	Dynamics of harpooning studied by transition state spectroscopy. II. Li??FH. *Journal of Chemical Physics*, **2000**, 113, 9897-9900	3.9	28
65	Parallelization of a legacy research program using OpenMP. *ACM SIGPLAN Fortran Forum*, **2000**, 19, 16-23	0.6	

64	Bound and quasi-bound states of the Li?FH van der Waals molecule **2000**, 80, 916		1
63	Complete set of solutions of the generalized Bloch equation **2000**, 80, 757		1
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