Piotr Piecuch

List of Publications by Citations

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	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
224	Renormalized coupled-cluster methods exploiting left eigenstates of the similarity-transformed Hamiltonian. *Journal of Chemical Physics*, **2005**, 123, 224105	3.9	364
223	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
222	A state-selective multireference coupled-cluster theory employing the single-reference formalism. *Journal of Chemical Physics*, **1993**, 99, 1875-1900	3.9	286
221	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
220	Recent developments in the general atomic and molecular electronic structure system. *Journal of Chemical Physics*, **2020**, 152, 154102	3.9	274
219	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
218	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
217	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	3.9	219
216	Application of Hilbert-space coupled-cluster theory to simple (H2)2 model systems: Planar models. *Physical Review A*, **1993**, 47, 2738-2782	2.6	201
215	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
214	Renormalized CCSD(T) and CCSD(TQ) approaches: Dissociation of the N2 triple bond. *Journal of Chemical Physics*, **2000**, 113, 5644-5652	3.9	193
213	State-selective multireference coupled-cluster theory employing the single-reference formalism: Implementation and application to the H8 model system. *Journal of Chemical Physics*, **1994**, 100, 5792-5809	3.9	178
212	Local correlation calculations using standard and renormalized coupled-cluster approaches. *Journal of Chemical Physics*, **2009**, 131, 114109	3.9	177
211	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
210	Single-reference, size-extensive, non-iterative coupled-cluster approaches to bond breaking and biradicals. *Chemical Physics Letters*, **2006**, 418, 467-474	2.5	171
209	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

208	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
207	Combined coupled-cluster and many-body perturbation theories. *Journal of Chemical Physics*, **2004**, 121, 12197-207	3.9	156
206	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
205	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
204	Coupled-cluster theory for three-body Hamiltonians. *Physical Review C*, **2007**, 76,	2.7	129
203	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	2.1	115
202	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
201	Orthogonally spin-adapted multi-reference Hilbert space coupled-cluster formalism: diagrammatic formulation. *Theoretica Chimica Acta*, **1992**, 83, 69-103		111
200	Application of Hilbert-space coupled-cluster theory to simple (H2)2 model systems. II. Nonplanar models. *Physical Review A*, **1994**, 49, 3479-3514	2.6	110
199	Coupled cluster calculations of ground and excited states of nuclei. *Physical Review Letters*, **2004**, 92, 132501	7.4	109
198	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
197	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	2.6	108
196	Orthogonally spin-adapted state-universal coupled-cluster formalism: Implementation of the complete two-reference theory including cubic and quartic coupling terms. *Journal of Chemical Physics*, **1994**, 101, 5875-5890	3.9	107
195	Thermochemical kinetics for multireference systems: addition reactions of ozone. *Journal of Physical Chemistry A*, **2009**, 113, 5786-99	2.8	106
194	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
193	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
192	Coupled cluster approaches with an approximate account of triexcitations and the optimized inner projection technique. *Theoretica Chimica Acta*, **1990**, 78, 65-128		101
191	EOMXCC: A New Coupled-Cluster Method for Electronic Excited States. *Advances in Quantum Chemistry*, **1999**, 34, 295-380	1.4	99

190	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
189	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
188	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
187	Extensive generalization of renormalized coupled-cluster methods. *Journal of Chemical Physics*, **2005**, 122, 074107	3.9	94
186	Improved computational strategy for the state-selective coupled-cluster theory with semi-internal triexcited clusters: Potential energy surface of the HF molecule. *Journal of Chemical Physics*, **1995**, 103, 9331-9346	3.9	93
185	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
184	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
183	Ab-initio coupled-cluster study of 16O. *Physical Review Letters*, **2005**, 94, 212501	7.4	90
182	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
181	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	3.9	84
180	Complete set of solutions of multireference coupled-cluster equations: The state-universal formalism. *Physical Review A*, **2000**, 61,	2.6	82
179	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
178	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
177	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
176	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
175	Molecular quadrupole moment functions of HF and N2. I. Ab initio linear-response coupled-cluster results. *Journal of Chemical Physics*, **1996**, 104, 4699-4715	3.9	74
174	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
173	Active-space coupled-cluster methods. *Molecular Physics*, **2010**, 108, 2987-3015	1.7	68

172	Breaking bonds with the state-selective multireference coupled-cluster method employing the single-reference formalism. *Journal of Chemical Physics*, **1995**, 102, 898-904	3.9	65
171	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
170	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
169	Coupled-cluster calculations for valence systems around O16. *Physical Review C*, **2006**, 74,	2.7	61
168	In Search of the Relationship between Multiple Solutions Characterizing Coupled-Cluster Theories. *Computational Chemistry - Reviews of Current Trends*, **2000**, 1-104		60
167	Breaking bonds with the left eigenstate completely renormalized coupled-cluster method. *Journal of Chemical Physics*, **2007**, 127, 174106	3.9	59
166	Active-space coupled-cluster study of electronic states of Be3. *Journal of Chemical Physics*, **2005**, 123, 074319	3.9	58
165	Comparison of low-order multireference many-body perturbation theories. *Journal of Chemical Physics*, **2005**, 122, 134105	3.9	58
164	Converging High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions. *Physical Review Letters*, **2017**, 119, 223003	7.4	56
163	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
162	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
161	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	2.5	55
160	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	3.3	55
159	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
158	New classes of non-iterative energy corrections to multi-reference coupled-cluster energies. *Molecular Physics*, **2004**, 102, 2425-2449	1.7	54
157	State-selective multireference coupled-cluster theory: In pursuit of property calculation. *Journal of Chemical Physics*, **1996**, 104, 6582-6589	3.9	54
156	Method of moments approach and coupled cluster theory. *Theoretica Chimica Acta*, **1991**, 80, 223-243		54
155	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

154	The state-selective coupled cluster method for quasi-degenerate electronic states. *Molecular Physics*, **1998**, 94, 225-234	1.7	53
153	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	2.5	52
152	The Ground State Electronic Energy of Benzene. *Journal of Physical Chemistry Letters*, **2020**, 11, 8922-8929	6.4	52
151	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
150	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
149	Orthogonally spin-adapted single-reference coupled-cluster formalism: Linear response calculation of static properties. *Journal of Chemical Physics*, **1995**, 102, 6511-6524	3.9	51
148	Experimental and theoretical UV characterizations of acetylacetone and its isomers. *Journal of Physical Chemistry A*, **2006**, 110, 3920-6	2.8	50
147	Potential energy surfaces of NaFH. *Journal of Chemical Physics*, **1998**, 108, 5349-5377	3.9	50
146	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
145	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
144	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
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142	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
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	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
139	The nonadditive interactions in the Ar2HF and Ar2HCl clusters: An ab initio study. *Journal of Chemical Physics*, **1993**, 99, 6732-6741	3.9	46
138	Solving the single-reference coupled-cluster equations involving highly excited clusters in quasidegenerate situations. *Journal of Chemical Physics*, **1994**, 100, 5857-5869	3.9	46
137	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

136	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
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134	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	2.5	43
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131	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
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128	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	2.5	39
127	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
126	Property Evaluation Using the Two-Reference State-Universal Coupled-Cluster Method. *The Journal of Physical Chemistry*, **1995**, 99, 15354-15368		38
125	Electron correlation in one dimension: Coupled cluster approaches to cyclic polyene electron models. *International Journal of Quantum Chemistry*, **1992**, 42, 135-164	2.1	38
124	Complete set of solutions of the generalized Bloch equation. *International Journal of Quantum Chemistry*, **2000**, 80, 757-781	2.1	37
123	The photoabsorption spectrum of Na?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	3.9	37
122	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
121	Exactness of two-body cluster expansions in many-body quantum theory. *Physical Review Letters*, **2003**, 90, 113001	7.4	36
120	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	2.1	36
119	Method of moments for the continuous transition between the Brillouin Wigner-type and Rayleigh Schr inger-type multireference coupled cluster theories. *Molecular Physics*, **2009**, 107, 1209-1221	1.7	34

118	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
117	Benchmarking the completely renormalised equation-of-motion coupled-cluster approaches for vertical excitation energies. *Molecular Physics*, **2015**, 113, 3085-3127	1.7	32
116	State-selective multi-reference coupled-cluster theory employing the single-reference formalism: Application to an excited state of H8. *Journal of Chemical Physics*, **1995**, 102, 3301-3306	3.9	32
115	Dynamics of harpooning studied by transition state spectroscopy Na□□FH. *Faraday Discussions*, **1997**, 108, 411-425	3.6	31
114	Extrapolating potential energy surfaces by scaling electron correlation at a single geometry. *Chemical Physics Letters*, **2006**, 430, 448-453	2.5	31
113	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
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111	Renormalized Coupled-Cluster Calculations of Reactive Potential Energy Surfaces: The BeFH System□ *Journal of Physical Chemistry A*, **2004**, 108, 8878-8893	2.8	29
110	Method of moments of coupled-cluster equations: The quasivariational and quadratic approximations. *Journal of Chemical Physics*, **2003**, 119, 2951-2962	3.9	28
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108	Dynamics of harpooning studied by transition state spectroscopy. II. Li??FH. *Journal of Chemical Physics*, **2000**, 113, 9897-9900	3.9	28
107	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
106	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
105	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
104	Coupled-cluster and configuration-interaction calculations for heavy nuclei. *Physical Review Letters*, **2007**, 98, 112501	7.4	27
103	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
102	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
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100	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
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97	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
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95	Communication: Determining the lowest-energy isomer of Au8: 2D, or not 2D. *Journal of Chemical Physics*, **2013**, 139, 091101	3.9	22
94	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
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92	Extrapolating potential energy surfaces by scaling electron correlation: isomerization of bicyclobutane to butadiene. *Journal of Chemical Physics*, **2008**, 128, 154116	3.9	21
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89	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
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87	Bound and quasibound states of the Na?FH van der Waals molecule. *Journal of Chemical Physics*, **2000**, 112, 189-202	3.9	19
86	Molecular quadrupole moment functions of HF and N2. II. Rovibrational effects. *Journal of Chemical Physics*, **1996**, 104, 4716-4727	3.9	19
85	Spherical tensor theory of long-range interactions between two molecules. *International Journal of Quantum Chemistry*, **1984**, 25, 449-473	2.1	19
84	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
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82	Theoretical studies of lithium bonding in lithium chloride/aliphatic amine complexes. *Chemical Physics*, **1985**, 94, 55-63	2.3	18
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80	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
79	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
78	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	2.6	17
77	Nuclear Structure Calculations with Coupled Cluster Methods from Quantum Chemistry. *Nuclear Physics A*, **2005**, 752, 299-308	1.3	16
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75	Diffusion of Atomic Oxygen on the Si(100) Surface. *Journal of Physical Chemistry C*, **2010**, 114, 12649-12658	3.8	15
74	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
73	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
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