Markus Reiher

List of Publications by Year
in descending order

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341 papers	24,095 citations	10373 72 h-index	10724 138 g-index
403 all docs	403 docs citations	403 times ranked	14369 citing authors

#	Article	IF	Citations
1	MOLCAS 7: The Next Generation. Journal of Computational Chemistry, 2010, 31, 224-247.	1.5	1,485
2	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. Journal of Computational Chemistry, 2016, 37, 506-541.	1.5	1,317
3	Reparameterization of hybrid functionals based on energy differences of states of different multiplicity. Theoretical Chemistry Accounts, 2001, 107, 48-55.	0.5	1,240
4	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	2.3	661
5	The generalized Douglasâ€“Kroll transformation. Journal of Chemical Physics, 2002, 117, 9215-9226.	1.2	638
6	Exact decoupling of the Dirac Hamiltonian. II. The generalized Douglasâ€“Krollâ€“Hess transformation up to arbitrary order. Journal of Chemical Physics, 2004, 121, 10945.	1.2	538
7	Assertion and validation of the performance of the B3LYPâ‹† functional for the first transition metal row and the G2 test set. Journal of Chemical Physics, 2002, 117, 4729-4737.	1.2	534
8	Quantum chemical calculation of vibrational spectra of large molecules?Raman and IR spectra for Buckminsterfullerene. Journal of Computational Chemistry, 2002, 23, 895-910.	1.5	506
9	Exact decoupling of the Dirac Hamiltonian. I. General theory. Journal of Chemical Physics, 2004, 121, 2037-2047.	1.2	455
10	Theoretical Study of the Fe(phen)2(NCS)2Spin-Crossover Complex with Reparametrized Density Functionals. Inorganic Chemistry, 2002, 41, 6928-6935.	1.9	411
11	Elucidating reaction mechanisms on quantum computers. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 7555-7560.	3.3	401
12	Modern quantum chemistry with [Open]Molcas. Journal of Chemical Physics, 2020, 152, 214117.	1.2	281
13	Exact decoupling of the relativistic Fock operator. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	238
14	Automated Selection of Active Orbital Spaces. Journal of Chemical Theory and Computation, 2016, 12, 1760-1771.	2.3	237
15	Douglasâ€“Krollâ€“Hess Theory: a relativistic electrons-only theory for chemistry. Theoretical Chemistry Accounts, 2006, 116, 241-252.	0.5	227
16	Spin in densityâ€functional theory. International Journal of Quantum Chemistry, 2012, 112, 3661-3684.	1.0	185
17	New Benchmark Set of Transition-Metal Coordination Reactions for the Assessment of Density Functionals. Journal of Chemical Theory and Computation, 2014, 10, 3092-3103.	2.3	181
18	Cooperative Lightâ€Activated Iodine and Photoredox Catalysis for the Amination of Câ^'H Bonds. Angewandte Chemie - International Edition, 2017, 56, 8004-8008.	7.2	181

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19	The Secret of Dimethyl Sulfoxideâ^'Water Mixtures. A Quantum Chemical Study of 1DMSOâ^'nWater Clusters. Journal of the American Chemical Society, 2002, 124, 6206-6215.	6.6	174
20	Accurate frozen-density embedding potentials as a first step towards a subsystem description of covalent bonds. Journal of Chemical Physics, 2010, 132, 164101.	1.2	172
21	Combined Spectroscopic and Theoretical Evidence for a Persistent End-On Copper Superoxo Complex. Angewandte Chemie - International Edition, 2004, 43, 4360-4363.	7.2	162
22	The Density Matrix Renormalization Group Algorithm in Quantum Chemistry. Zeitschrift Fur Physikalische Chemie, 2010, 224, 583-599.	1.4	162
23	Density matrix renormalization group calculations on relative energies of transition metal complexes and clusters. Journal of Chemical Physics, 2008, 128, 014104.	1.2	158
24	An efficient implementation of two-component relativistic exact-decoupling methods for large molecules. Journal of Chemical Physics, 2013, 138, 184105.	1.2	158
25	Heavy Grignard Reagents: Challenges and Possibilities of Aryl Alkaline Earth Metal Compounds. Chemistry - A European Journal, 2007, 13, 6292-6306.	1.7	157
26	Quantum-information analysis of electronic states of different molecular structures. Physical Review A, 2011, 83, .	1.0	152
27	The density matrix renormalization group in chemistry and molecular physics: Recent developments and new challenges. Journal of Chemical Physics, 2020, 152, 040903.	1.2	152
28	Stable â€œInverseâ€•Sandwich Complex with Unprecedented Organocalcium(I): Crystal Structures of [(thf)₂Mg(Br)-C₆H₂-2,4,6-Ph₃] and [(thf)₃Ca{Ì¼-C₆H₃-1,3,5-Ph₃}Ca(thf)₃]. Journal of the American Chemical Society, 2009, 131, 2977-2985.	6.6	149
29	Entanglement Measures for Single- and Multireference Correlation Effects. Journal of Physical Chemistry Letters, 2012, 3, 3129-3135.	2.1	143
30	Exploration of Reaction Pathways and Chemical Transformation Networks. Journal of Physical Chemistry A, 2019, 123, 385-399.	1.1	141
31	Localizing normal modes in large molecules. Journal of Chemical Physics, 2009, 130, 084106.	1.2	140
32	Comparison of density functionals for differences between the high- (T2g5) and low- (A1g1) spin states of iron(II) compounds. IV. Results for the ferrous complexes [Fe(L)(â€¯NHS4â€™)]. Journal of Chemical Physics, 2005, 122, 234321.	1.2	127
33	An efficient matrix product operator representation of the quantum chemical Hamiltonian. Journal of Chemical Physics, 2015, 143, 244118.	1.2	127
34	Heuristics-Guided Exploration of Reaction Mechanisms. Journal of Chemical Theory and Computation, 2015, 11, 5712-5722.	2.3	127
35	Convergence behavior of the density-matrix renormalization group algorithm for optimized orbital orderings. Journal of Chemical Physics, 2005, 122, 024107.	1.2	121
36	New electron correlation theories for transition metal chemistry. Physical Chemistry Chemical Physics, 2011, 13, 6750.	1.3	120

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37	Relativistic Douglasâ€“Krollâ€“Hess theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 139-149.	6.2	120
38	Estimation of the Vibrational Contribution to the Entropy Change Associated with the Low- to High-Spin Transition in Fe(phen)2(NCS)2 Complexes:â€‰ Results Obtained by IR and Raman Spectroscopy and DFT Calculations. Journal of Physical Chemistry A, 2002, 106, 12024-12034.	1.1	119
39	Intrinsic Dinitrogen Activation at Bare Metal Atoms. Angewandte Chemie - International Edition, 2006, 45, 6264-6288.	7.2	117
40	First-Principles Investigation of the Schrock Mechanism of Dinitrogen Reduction Employing the Full HIPTN₃N Ligand. Inorganic Chemistry, 2008, 47, 3634-3650.	1.9	111
41	A mode-selective quantum chemical method for tracking molecular vibrations applied to functionalized carbon nanotubes. Journal of Chemical Physics, 2003, 118, 1634-1641.	1.2	106
42	Basis Set and Density Functional Dependence of Vibrational Raman Optical Activity Calculations. Journal of Physical Chemistry A, 2005, 109, 7567-7574.	1.1	105
43	The Exploration of Chemical Reaction Networks. Annual Review of Physical Chemistry, 2020, 71, 121-142.	4.8	103
44	Orbital Entanglement in Bond-Formation Processes. Journal of Chemical Theory and Computation, 2013, 9, 2959-2973.	2.3	98
45	Properties of WAu12. Physical Chemistry Chemical Physics, 2004, 6, 11-22.	1.3	97
46	Can DFT Accurately Predict Spin Densities? Analysis of Discrepancies in Iron Nitrosyl Complexes. Journal of Chemical Theory and Computation, 2011, 7, 2740-2752.	2.3	96
47	Quantum computing enhanced computational catalysis. Physical Review Research, 2021, 3, .	1.3	96
48	Theoretical Study of Catalytic Dinitrogen Reduction under Mild Conditions. Inorganic Chemistry, 2005, 44, 9640-9642.	1.9	94
49	New Approaches for ab initio Calculations of Molecules with Strong Electron Correlation. Chimia, 2016, 70, 244.	0.3	94
50	Capture and characterization of a reactive haemâ€“carbenoid complex in an artificial metalloenzyme. Nature Catalysis, 2018, 1, 578-584.	16.1	93
51	Assignment of Vibrational Spectra of 1,10-Phenanthroline by Comparison with Frequencies and Raman Intensities from Density Functional Calculations. Journal of Physical Chemistry A, 2004, 108, 734-742.	1.1	91
52	Calculation of electric-field gradients based on higher-order generalized Douglasâ€“Kroll transformations. Journal of Chemical Physics, 2005, 122, 204107.	1.2	89
53	Local relativistic exact decoupling. Journal of Chemical Physics, 2012, 136, 244108.	1.2	88
54	Multireference Perturbation Theory with Cholesky Decomposition for the Density Matrix Renormalization Group. Journal of Chemical Theory and Computation, 2017, 13, 451-459.	2.3	88

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55	The Matter Simulation (R)evolution. ACS Central Science, 2018, 4, 144-152.	5.3	88
56	Comparative analysis of local spin definitions. Journal of Chemical Physics, 2005, 122, 034102.	1.2	87
57	Hydrogenases and oxygen. Chemical Science, 2012, 3, 1739.	3.7	87
58	Context-Driven Exploration of Complex Chemical Reaction Networks. Journal of Chemical Theory and Computation, 2017, 13, 6108-6119.	2.3	87
59	Density matrix renormalization group with efficient dynamical electron correlation through range separation. Journal of Chemical Physics, 2015, 142, 224108.	1.2	86
60	Gas-Phase Câˆ’H and Nâˆ’H Bond Activation by a High Valent Nitrido-Iron Dication and ã€ˆNHã€‰-Transfer to Activated Olefins. Journal of the American Chemical Society, 2008, 130, 4285-4294.	6.6	85
61	Selection of active spaces for multiconfigurational wavefunctions. Journal of Chemical Physics, 2015, 142, 244104.	1.2	84
62	Engineering Molecular Iodine Catalysis for Alkylâ€“Nitrogen Bond Formation. ACS Catalysis, 2018, 8, 3918-3925.	5.5	83
63	Tetracycline and derivativesâ€”assignment of IR and Raman spectra via DFT calculations. Physical Chemistry Chemical Physics, 2003, 5, 1149-1157.	1.3	82
64	Complete-graph tensor network states: a new fermionic wave function ansatz for molecules. New Journal of Physics, 2010, 12, 103008.	1.2	82
65	Exact decoupling of the Dirac Hamiltonian. III. Molecular properties. Journal of Chemical Physics, 2006, 124, 064102.	1.2	80
66	Accurate ab Initio Spin Densities. Journal of Chemical Theory and Computation, 2012, 8, 1970-1982.	2.3	79
67	Communication: Four-component density matrix renormalization group. Journal of Chemical Physics, 2014, 140, 041101.	1.2	79
68	Binding N2, N2H2, N2H4, and NH3 to Transition-Metal Sulfur Sites: Modeling Potential Intermediates of Biological N2 Fixation. Chemistry - A European Journal, 2004, 10, 819-830.	1.7	78
69	The Delicate Balance of Static and Dynamic Electron Correlation. Journal of Chemical Theory and Computation, 2016, 12, 3764-3773.	2.3	78
70	Decomposition of density matrix renormalization group states into a Slater determinant basis. Journal of Chemical Physics, 2007, 126, 244109.	1.2	77
71	Theoretical Raman Optical Activity Study of the Î² Domain of Rat Metallothionein. Journal of Physical Chemistry B, 2010, 114, 1057-1063.	1.2	76
72	Nitrous Oxide as a Hydrogen Acceptor for the Dehydrogenative Coupling of Alcohols. Angewandte Chemie - International Edition, 2016, 55, 1854-1858.	7.2	76

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73	Stoichiometric Reactions of Enamines Derived from Diphenylprolinol Silyl Ethers with Nitro Olefins and Lessons for the Corresponding Organocatalytic Conversions â€“ a Survey. Helvetica Chimica Acta, 2013, 96, 799-852.	1.0	75
74	Formation of a Nickelâ^'Methyl Species in Methyl-Coenzyme M Reductase, an Enzyme Catalyzing Methane Formation. Journal of the American Chemical Society, 2007, 129, 11028-11029.	6.6	74
75	Spin-adapted matrix product states and operators. Journal of Chemical Physics, 2016, 144, 134101.	1.2	74
76	Analysis of Secondary Structure Effects on the IR and Raman Spectra of Polypeptides in Terms of Localized Vibrations. Journal of Physical Chemistry B, 2009, 113, 6558-6573.	1.2	72
77	Nitrogen Fixation under Mild Ambient Conditions: Part Iâ€”The Initial Dissociation/Association Step at Molybdenum Triamidoamine Complexes. Chemistry - A European Journal, 2005, 11, 7448-7460.	1.7	71
78	Chirality-Induced Switch in Hydrogen-Bond Topology: Tetrameric Methyl Lactate Clusters in the Gas Phase. Angewandte Chemie - International Edition, 2006, 45, 3440-3445.	7.2	71
79	Can Raman Optical Activity Separate Axial from Local Chirality? A Theoretical Study of Helical Deca-Alanine. ChemPhysChem, 2006, 7, 2189-2196.	1.0	71
80	Systematic Error Estimation for Chemical Reaction Energies. Journal of Chemical Theory and Computation, 2016, 12, 2762-2773.	2.3	71
81	Relativistic DMRG calculations on the curve crossing of cesium hydride. Journal of Chemical Physics, 2005, 123, 184105.	1.2	69
82	Molecular structure calculations: A unified quantum mechanical description of electrons and nuclei using explicitly correlated Gaussian functions and the global vector representation. Journal of Chemical Physics, 2012, 137, 024104.	1.2	69
83	On the definition of local spin in relativistic and nonrelativistic quantum chemistry. Faraday Discussions, 2007, 135, 97-124.	1.6	68
84	A Nickel Hydride Complex in the Active Site of Methyl-Coenzyme M Reductase: Implications for the Catalytic Cycle. Journal of the American Chemical Society, 2008, 130, 10907-10920.	6.6	68
85	Isoelectronic Arduengo-Type Carbene Analogues with the Group IIIa Elements Boron, Aluminum, Gallium, and Indium. , 1998, 1998, 305-310.		67
86	Understanding the Signatures of Secondaryâ€Structure Elements in Proteins with Raman Optical Activity Spectroscopy. Chemistry - A European Journal, 2009, 15, 13491-13508.	1.7	67
87	A stable phosphanyl phosphaketene and its reactivity. Dalton Transactions, 2015, 44, 6431-6438.	1.6	67
88	Finding a needle in a haystack: direct determination of vibrational signatures in complex systems. New Journal of Chemistry, 2007, 31, 818.	1.4	66
89	Analysis of electron density distributions from subsystem density functional theory applied to coordination bonds. Chemical Physics Letters, 2008, 461, 353-359.	1.2	66
90	Large-Scale Quantum Dynamics with Matrix Product States. Journal of Chemical Theory and Computation, 2019, 15, 3481-3498.	2.3	66

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91	Relativistic Effects on the Topology of the Electron Density. Journal of Chemical Theory and Computation, 2007, 3, 2182-2197.	2.3	65
92	Training Neural Nets To Learn Reactive Potential Energy Surfaces Using Interactive Quantum Chemistry in Virtual Reality. Journal of Physical Chemistry A, 2019, 123, 4486-4499.	1.1	65
93	Trinuclear Copper(II) Complexes Derived from Schiff-Base Ligands Based on a 6-Amino-6-deoxyglucopyranoside:â€‰ Structural and Magnetic Characterization. Inorganic Chemistry, 2006, 45, 10066-10076.	1.9	64
94	Analytic high-order Douglas-Kroll-Hess electric field gradients. Journal of Chemical Physics, 2007, 127, 074105.	1.2	64
95	Raman optical activity spectra of chiral transition metal complexes. Chemical Physics, 2008, 346, 212-223.	0.9	64
96	Uncertainty quantification for quantum chemical models of complex reaction networks. Faraday Discussions, 2016, 195, 497-520.	1.6	64
97	Kooperative Lichtâ€aktivierte Iodâ€•und Photoredoxâ€Katalyse zur Aminierung von Câ€Hâ€Bindungen. Angewandte Chemie, 2017, 129, 8117-8121.	1.6	63
98	Automated Identification of Relevant Frontier Orbitals for Chemical Compounds and Processes. Chimia, 2017, 71, 170.	0.3	63
99	Two-Component Relativistic Calculations of Electric-Field Gradients Using Exact Decoupling Methods: Spinâ€“orbit and Picture-Change Effects. Journal of Chemical Theory and Computation, 2012, 8, 4239-4248.	2.3	62
100	Hydrogen Spillover to Nonreducible Supports. Journal of Physical Chemistry C, 2012, 116, 14274-14283.	1.5	62
101	Calculation of Ligand Dissociation Energies in Large Transition-Metal Complexes. Journal of Chemical Theory and Computation, 2018, 14, 2456-2468.	2.3	62
102	Error-Controlled Exploration of Chemical Reaction Networks with Gaussian Processes. Journal of Chemical Theory and Computation, 2018, 14, 5238-5248.	2.3	62
103	Fluorescence kinetics of aqueous solutions of tetracycline and its complexes with Mg2+ and Ca2+This paper is dedicated to Professor Fred Lewis on the event of his 60th birthday.. Photochemical and Photobiological Sciences, 2003, 2, 1107.	1.6	61
104	Synthesis of Chiral Self-Assembling Rhombs and Their Characterization in Solution, in the Gas Phase, and at the Liquidâ^'Solid Interface. Journal of the American Chemical Society, 2005, 127, 17672-17685.	6.6	61
105	MÃ¶ssbauer spectroscopy for heavy elements: a relativistic benchmark study of mercury. Theoretical Chemistry Accounts, 2011, 129, 631-650.	0.5	61
106	Quantum Chemical Calculation of Raman Intensities for Large Molecules: The Photoisomerization of [{Feâ€˜S4â€™(PR3)}2(N2H2)] (â€˜S4â€™2â^'= 1,2-bis(2-Mercaptophenylthio)-Ethane(2â^')). Zeitschrift Fur Physikalische Chemie, 2003, 217, 91-104.	1.1	60
107	Second-Order Self-Consistent-Field Density-Matrix Renormalization Group. Journal of Chemical Theory and Computation, 2017, 13, 2533-2549.	2.3	60
108	<scp>autoCAS</scp>: A Program for Fully Automated Multiconfigurational Calculations. Journal of Computational Chemistry, 2019, 40, 2216-2226.	1.5	60

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109	M<scp>O</scp>V<scp>I</scp>P<scp>AC</scp>: Vibrational spectroscopy with a robust metaâ€program for massively parallel standard and inverse calculations. Journal of Computational Chemistry, 2012, 33, 2186-2198.	1.5	59
110	Exact decoupling of the Dirac Hamiltonian. IV. Automated evaluation of molecular properties within the Douglas-Kroll-Hess theory up to arbitrary order. Journal of Chemical Physics, 2006, 124, 064103.	1.2	58
111	Ligands for Dinitrogen Fixation at Schrock-Type Catalysts. Inorganic Chemistry, 2009, 48, 1638-1648.	1.9	58
112	Orbital entanglement and CASSCF analysis of the Ruâ€“NO bond in a Ruthenium nitrosyl complex. Physical Chemistry Chemical Physics, 2015, 17, 14383-14392.	1.3	58
113	Stabilization of diazene in Fe(II)-sulfur model complexes relevant for nitrogenase activity. I. A new approach to the evaluation of intramolecular hydrogen bond energies. Theoretical Chemistry Accounts, 2001, 106, 379-392.	0.5	57
114	The First Photoexcitation Step of Ruthenium-Based Models for Artificial Photosynthesis Highlighted by Resonance Raman Spectroscopy. Journal of Physical Chemistry B, 2007, 111, 6078-6087.	1.2	57
115	The Electronic Structure of the Tris(ethylene) Complexes [M(C₂H₄)₃] (M=Ni, Pd, and Pt): A Combined Experimental and Theoretical Study. Chemistry - A European Journal, 2007, 13, 10078-10087.	1.7	57
116	Predictors for gases of high electrical strength. IEEE Transactions on Dielectrics and Electrical Insulation, 2013, 20, 856-863.	1.8	57
117	First-Principles Approach to Vibrational Spectroscopy of Biomolecules. , 2006, , 85-132.		56
118	THF Solvates of Extremely Soluble Bis(2,4,6-trimethylphenyl)calcium and Tris(2,6-dimethoxyphenyl)dicalcium Iodide. Angewandte Chemie - International Edition, 2007, 46, 1618-1623.	7.2	56
119	Topological analysis of electron densities from Kohn-Sham and subsystem density functional theory. Journal of Chemical Physics, 2008, 128, 044114.	1.2	56
120	A Theoretical Challenge: Transition-Metal Compounds. Chimia, 2009, 63, 140.	0.3	55
121	Subvalent Organometallic Compounds of the Alkaline Earth Metals in Low Oxidation States. European Journal of Inorganic Chemistry, 2010, 2010, 197-216.	1.0	55
122	Enhancement and de-enhancement effects in vibrational resonance Raman optical activity. Journal of Chemical Physics, 2010, 132, 044113.	1.2	55
123	A Local-Mode Model for Understanding the Dependence of the Extended Amide III Vibrations on Protein Secondary Structure. Journal of Physical Chemistry B, 2010, 114, 10649-10660.	1.2	55
124	Dinuclear Diazene Iron and Ruthenium Complexes as Models for Studying Nitrogenase Activity. Chemistry - A European Journal, 2001, 7, 5195-5202.	1.7	54
125	Spin states in polynuclear clusters: The [Fe2O2] core of the methane monooxygenase active site. Journal of Computational Chemistry, 2006, 27, 1223-1239.	1.5	54
126	A theoretical study of spin states in Ni-S4 complexes and models of the [NiFe] hydrogenase active site. Journal of Biological Inorganic Chemistry, 2004, 9, 873-884.	1.1	52

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127	Targeting Intermediates of [FeFe]-Hydrogenase by CO and CN Vibrational Signatures. Inorganic Chemistry, 2011, 50, 3888-3900.	1.9	51
128	From Rare Gas Atoms to Fullerenes: Spherical Aromaticity Studied From the Point of View of Atomic Structure Theory. Chemistry - A European Journal, 2003, 9, 5442-5452.	1.7	50
129	A Stable Sixâ€Coordinate Intermediate in Ammoniaâ€“Dinitrogen Exchange at Schrock's Molybdenum Catalyst. Chemistry - A European Journal, 2009, 15, 5073-5082.	1.7	50
130	Theoretical Study of Dioxygen Induced Inhibition of [FeFe]-Hydrogenase. Inorganic Chemistry, 2009, 48, 7127-7140.	1.9	50
131	Hardware efficient quantum algorithms for vibrational structure calculations. Chemical Science, 2020, 11, 6842-6855.	3.7	50
132	Construction of environment states in quantum-chemical density-matrix renormalization group calculations. Journal of Chemical Physics, 2006, 124, 034103.	1.2	49
133	Organofluorosilanes as Model Compounds for ¹⁸Fâ€Labeled Siliconâ€Based PET Tracers and their Hydrolytic Stability: Experimental Data and Theoretical Calculations (PET=Positron Emission) Tj ETQq1 1 0.784314 rgBT /Overloc	1.7	49
134	On the emergence of molecular structure. Physical Review A, 2011, 83, .	1.0	49
135	Measuring multi-configurational character by orbital entanglement. Molecular Physics, 2017, 115, 2110-2119.	0.8	49
136	A Photochemical Activation Scheme of Inert Dinitrogen by Dinuclear RuII and FeII Complexes. Chemistry - A European Journal, 2004, 10, 4443-4453.	1.7	48
137	Calculated Raman Optical Activity Signatures of Tryptophan Side Chains. ChemPhysChem, 2008, 9, 2177-2180.	1.0	48
138	Inaccessibility of the Î¼-hydride species in [FeFe] hydrogenases. Chemical Science, 2014, 5, 215-221.	3.7	48
139	Systematic microsolvation approach with a clusterâ€continuum scheme and conformational sampling. Journal of Computational Chemistry, 2020, 41, 1144-1155.	1.5	48
140	Calculated Raman Optical Activity Spectra of 1,6-Anhydro-Î²-<scp>d</scp>-glucopyranose. Journal of Physical Chemistry A, 2009, 113, 8268-8277.	1.1	47
141	Regioselectivity of H Cluster Oxidation. Journal of the American Chemical Society, 2011, 133, 20588-20603.	6.6	47
142	Inverse quantum chemistry: Concepts and strategies for rational compound design. International Journal of Quantum Chemistry, 2014, 114, 823-837.	1.0	47
143	Interactive Chemical Reactivity Exploration. ChemPhysChem, 2014, 15, 3301-3319.	1.0	47
144	Reliable Estimation of Prediction Uncertainty for Physicochemical Property Models. Journal of Chemical Theory and Computation, 2017, 13, 3297-3317.	2.3	47

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145	The Douglasâ€“Krollâ€“Hess electron density at an atomic nucleus. Chemical Physics Letters, 2008, 465, 157-164.	1.2	46
146	Relevance of the Electric-Dipoleâ^'Electric-Quadrupole Contribution to Raman Optical Activity Spectra. Journal of Physical Chemistry B, 2008, 112, 2218-2232.	1.2	46
147	Analysis of the Cartesian Tensor Transfer Method for Calculating Vibrational Spectra of Polypeptides. Journal of Chemical Theory and Computation, 2011, 7, 1867-1881.	2.3	46
148	Construction of CASCI-type wave functions for very large active spaces. Journal of Chemical Physics, 2011, 134, 224101.	1.2	46
149	Unravelling the quantum-entanglement effect of noble gas coordination on the spin ground state of CUO. Physical Chemistry Chemical Physics, 2014, 16, 719-727.	1.3	46
150	Vibrational Density Matrix Renormalization Group. Journal of Chemical Theory and Computation, 2017, 13, 3764-3777.	2.3	46
151	Semiempirical molecular orbital models based on the neglect of diatomic differential overlap approximation. International Journal of Quantum Chemistry, 2018, 118, e25799.	1.0	46
152	Redox Activity of Oxo-Bridged Iridium Dimers in an N,O-Donor Environment: Characterization of Remarkably Stable Ir(IV,V) Complexes. Journal of the American Chemical Society, 2017, 139, 9672-9683.	6.6	45
153	Gaussian Process-Based Refinement of Dispersion Corrections. Journal of Chemical Theory and Computation, 2019, 15, 6046-6060.	2.3	44
154	Correlated ab initio calculations of spectroscopic parameters of SnO within the framework of the higher-order generalized Douglasâ€“Kroll transformation. Journal of Chemical Physics, 2004, 120, 8624-8631.	1.2	43
155	Extracting elements of molecular structure from the all-particle wave function. Journal of Chemical Physics, 2011, 135, 204302.	1.2	43
156	Investigation of the low-spin to high-spin transition in a novel [Fe(pmea)(NCS)2] complex by IR and Raman spectroscopy and DFT calculations. Journal of Raman Spectroscopy, 2006, 37, 108-122.	1.2	42
157	The Shell Structure of Atoms. Journal of Chemical Theory and Computation, 2008, 4, 286-296.	2.3	42
158	Catalytic synthesis of vinylphosphanes via calcium-mediated intermolecular hydrophosphanylation of alkynes and butadiynes. Journal of Organometallic Chemistry, 2011, 696, 216-227.	0.8	42
159	Hydrogen-activation mechanism of [Fe] hydrogenase revealed by multi-scale modeling. Chemical Science, 2014, 5, 4474-4482.	3.7	42
160	A Unifying Structural and Electronic Concept for Hmd and [FeFe] Hydrogenase Active Sites. Inorganic Chemistry, 2010, 49, 5818-5823.	1.9	40
161	Coupled-cluster Raman intensities: Assessment and comparison with multiconfiguration and density functional methods. Journal of Chemical Physics, 2002, 117, 8623-8633.	1.2	39
162	Metal thiolate complexes binding molecular nitrogen under mild conditions: [Î¼-N2{Ru(PiPr3)(N2Me2S2)}2], the first dinuclear example. Inorganica Chimica Acta, 2003, 348, 194-198.	1.2	39

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163	Convergence characteristics and efficiency of mode-tracking calculations on pre-selected molecular vibrations. Physical Chemistry Chemical Physics, 2004, 6, 4621.	1.3	39
164	Nuclear Quadrupole Moment of ¹¹⁹Sn. Journal of Physical Chemistry A, 2008, 112, 1666-1672.	1.1	39
165	Intensity tracking for theoretical infrared spectroscopy of large molecules. Journal of Chemical Physics, 2009, 130, 064105.	1.2	39
166	Intensityâ€Carrying Modes in Raman and Raman Optical Activity Spectroscopy. ChemPhysChem, 2009, 10, 2049-2057.	1.0	39
167	Quantum entanglement in carbonâ€“carbon, carbonâ€“phosphorus and siliconâ€“silicon bonds. Physical Chemistry Chemical Physics, 2014, 16, 8872-8880.	1.3	39
168	A Nonorthogonal State-Interaction Approach for Matrix Product State Wave Functions. Journal of Chemical Theory and Computation, 2016, 12, 5881-5894.	2.3	39
169	Studying chemical reactivity in a virtual environment. Faraday Discussions, 2014, 169, 89-118.	1.6	37
170	Spinâ€“Spin interactions in polynuclear transition-metal complexes. Chemical Physics Letters, 2008, 451, 301-308.	1.2	36
171	Selective calculation of high-intensity vibrations in molecular resonance Raman spectra. Journal of Chemical Physics, 2008, 129, 204103.	1.2	36
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