Markus Reiher

List of Publications by Year
in descending order

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	Heuristics and Uncertainty Quantification in Rational and Inverse Compound and Catalyst Design. , 2024, , 485-495.		0
2	Solvation Free Energies in Subsystem Density Functional Theory. Journal of Chemical Theory and Computation, 2022, 18, 723-740.	2.3	12
3	Quantum Proton Effects from Density Matrix Renormalization Group Calculations. Journal of Chemical Theory and Computation, 2022, 18, 234-250.	2.3	10
4	Autonomous Reaction Network Exploration in Homogeneous and Heterogeneous Catalysis. Topics in Catalysis, 2022, 65, 6-39.	1.3	27
5	The apparently unreactive substrate facilitates the electron transfer for dioxygen activation in Rieske dioxygenases. Chemistry - A European Journal, 2022, , .	1.7	6
6	Expansive Quantum Mechanical Exploration of Chemical Reaction Paths. Accounts of Chemical Research, 2022, 55, 35-43.	7.6	14
7	Excited-State DMRG Made Simple with FEAST. Journal of Chemical Theory and Computation, 2022, 18, 415-430.	2.3	13
8	Prospects of quantum computing for molecular sciences. Materials Theory, 2022, 6, .	2.2	21
9	Moleculeâ€Specific Uncertainty Quantification in Quantum Chemical Studies. Israel Journal of Chemistry, 2022, 62, .	1.0	16
10	The transferability limits of static benchmarks. Physical Chemistry Chemical Physics, 2022, 24, 14692-14698.	1.3	8
11	The (not so) simple prediction of enantioselectivity â€“ a pipeline for high-fidelity computations. Chemical Science, 2022, 13, 6858-6864.	3.7	6
12	Explicitly Correlated Electronic Structure Calculations with Transcorrelated Matrix Product Operators. Journal of Chemical Theory and Computation, 2022, 18, 4203-4217.	2.3	9
13	Immersive Interactive Quantum Mechanics for Teaching and Learning Chemistry. Chimia, 2021, 75, 45.	0.3	8
14	On the Predictive Power of Chemical Concepts. Chimia, 2021, 75, 311.	0.3	10
15	Automated Construction of Quantumâ€“Classical Hybrid Models. Journal of Chemical Theory and Computation, 2021, 17, 3797-3813.	2.3	18
16	Charge-Transfer-Induced Predissociation in Rydberg States of Molecular Cations: MgAr+. Journal of Physical Chemistry A, 2021, 125, 6681-6696.	1.1	2
17	Quantum computing enhanced computational catalysis. Physical Review Research, 2021, 3, .	1.3	96
18	Transcorrelated density matrix renormalization group. Journal of Chemical Physics, 2020, 153, 164115.	1.2	23

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19	Analytically projected, rotationally symmetric, explicitly correlated Gaussian functions with one-axis-shifted centers. Physical Review A, 2020, 102, .	1.0	1
20	Complete characterization of the 3p Rydberg complex of a molecular ion: MgAr+. I. Observation of the Mg(3pÏƒ)Ar+ B+ state and determination of its structure and dynamics. Journal of Chemical Physics, 2020, 153, 074310.	1.2	11
21	Nuclear-electronic all-particle density matrix renormalization group. Journal of Chemical Physics, 2020, 152, 204103.	1.2	16
22	Hardware efficient quantum algorithms for vibrational structure calculations. Chemical Science, 2020, 11, 6842-6855.	3.7	50
23	Modern quantum chemistry with [Open]Molcas. Journal of Chemical Physics, 2020, 152, 214117.	1.2	281
24	Semiclassical Dispersion Corrections Efficiently Improve Multiconfigurational Theory with Short-Range Density-Functional Dynamic Correlation. Journal of Physical Chemistry A, 2020, 124, 2834-2841.	1.1	4
25	M<scp>olassembler</scp>: Molecular Graph Construction, Modification, and Conformer Generation for Inorganic and Organic Molecules. Journal of Chemical Information and Modeling, 2020, 60, 3884-3900.	2.5	36
26	The Exploration of Chemical Reaction Networks. Annual Review of Physical Chemistry, 2020, 71, 121-142.	4.8	103
27	Self-Parametrizing System-Focused Atomistic Models. Journal of Chemical Theory and Computation, 2020, 16, 1646-1665.	2.3	22
28	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
29	Systematic microsolvation approach with a clusterâ€continuum scheme and conformational sampling. Journal of Computational Chemistry, 2020, 41, 1144-1155.	1.5	48
30	Tailored coupled cluster theory in varying correlation regimes. Journal of Chemical Physics, 2020, 153, 244113.	1.2	13
31	The electrostatic potential as a descriptor for the protonation propensity in automated exploration of reaction mechanisms. Faraday Discussions, 2019, 220, 443-463.	1.6	32
32	H 3 + as a five-body problem described with explicitly correlated Gaussian basis sets. Journal of Chemical Physics, 2019, 151, 154110.	1.2	12
33	Approximate Analytical Gradients and Nonadiabatic Couplings for the State-Average Density Matrix Renormalization Group Self-Consistent-Field Method. Journal of Chemical Theory and Computation, 2019, 15, 6724-6737.	2.3	17
34	Gaussian Process-Based Refinement of Dispersion Corrections. Journal of Chemical Theory and Computation, 2019, 15, 6046-6060.	2.3	44
35	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	2.3	661
36	<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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37	Large-Scale Quantum Dynamics with Matrix Product States. Journal of Chemical Theory and Computation, 2019, 15, 3481-3498.	2.3	66
38	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
39	Optimization of highly excited matrix product states with an application to vibrational spectroscopy. Journal of Chemical Physics, 2019, 150, 094113.	1.2	29
40	Understanding unusual element-element bond formation and activation: general discussion. Faraday Discussions, 2019, 220, 376-385.	1.6	0
41	Physical methods for mechanistic understanding: general discussion. Faraday Discussions, 2019, 220, 144-178.	1.6	0
42	Mechanistic insight into organic and industrial transformations: general discussion. Faraday Discussions, 2019, 220, 282-316.	1.6	8
43	Computational and theoretical approaches for mechanistic understanding: general discussion. Faraday Discussions, 2019, 220, 464-488.	1.6	3
44	Exploration of Reaction Pathways and Chemical Transformation Networks. Journal of Physical Chemistry A, 2019, 123, 385-399.	1.1	141
45	Mechanism Deduction from Noisy Chemical Reaction Networks. Journal of Chemical Theory and Computation, 2019, 15, 357-370.	2.3	31
46	Statistical Analysis of Semiclassical Dispersion Corrections. Journal of Chemical Theory and Computation, 2018, 14, 2480-2494.	2.3	25
47	Minimum Energy Paths and Transition States by Curve Optimization. Journal of Chemical Theory and Computation, 2018, 14, 3091-3099.	2.3	23
48	The Matter Simulation (R)evolution. ACS Central Science, 2018, 4, 144-152.	5.3	88
49	Structure and dynamics of the radical cation of ethane arising from the Jahnâ€“Teller and pseudo-Jahnâ€“Teller effects. Physical Chemistry Chemical Physics, 2018, 20, 1072-1081.	1.3	11
50	Calculation of Ligand Dissociation Energies in Large Transition-Metal Complexes. Journal of Chemical Theory and Computation, 2018, 14, 2456-2468.	2.3	62
51	Engineering Molecular Iodine Catalysis for Alkylâ€“Nitrogen Bond Formation. ACS Catalysis, 2018, 8, 3918-3925.	5.5	83
52	Integrated Reaction Path Processing from Sampled Structure Sequences. Journal of Chemical Theory and Computation, 2018, 14, 2052-2062.	2.3	10
53	Hydrogenâ€Bonded Networks: Molecular Recognition of Cyclic Alcohols in Enantiopure Allenoâ€Acetylenic Cage Receptors. Angewandte Chemie - International Edition, 2018, 57, 16296-16301.	7.2	8
54	Quantum system partitioning at the single-particle level. Journal of Chemical Physics, 2018, 149, 184104.	1.2	17

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55	WasserstoffbrÃ¼ckenâ€Netzwerke: molekulare Erkennung zyklischer Alkohole in enantiomerenreinen allenoâ€acetylenischen KÃfigrezeptoren. Angewandte Chemie, 2018, 130, 16534-16539.	1.6	1
56	Explicitly correlated Gaussian functions with shifted-center and projection techniques in pre-Bornâ€"Oppenheimer calculations. Journal of Chemical Physics, 2018, 149, 184105.	1.2	11
57	Semiempirical molecular orbital models based on the neglect of diatomic differential overlap approximation. International Journal of Quantum Chemistry, 2018, 118, e25799.	1.0	46
58	Comprehensive Analysis of the Neglect of Diatomic Differential Overlap Approximation. Journal of Chemical Theory and Computation, 2018, 14, 5169-5179.	2.3	18
59	Error-Controlled Exploration of Chemical Reaction Networks with Gaussian Processes. Journal of Chemical Theory and Computation, 2018, 14, 5238-5248.	2.3	62
60	Redoxâ€Active Chiroptical Switching in Monoâ€•and Bisâ€Iron Ethynylcarbo[6]helicenes Studied by Electronic and Vibrational Circular Dichroism and Resonance Raman Optical Activity. Chemistry - A European Journal, 2018, 24, 15067-15079.	1.7	24
61	Capture and characterization of a reactive haemâ€"carbenoid complex in an artificial metalloenzyme. Nature Catalysis, 2018, 1, 578-584.	16.1	93
62	Generalized elimination of the global translation from explicitly correlated Gaussian functions. Journal of Chemical Physics, 2018, 148, 084112.	1.2	11
63	Generalized Pauli constraints in small atoms. Physical Review A, 2018, 97, .	1.0	22
64	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
65	Measuring multi-configurational character by orbital entanglement. Molecular Physics, 2017, 115, 2110-2119.	0.8	49
66	Steering Orbital Optimization out of Local Minima and Saddle Points Toward Lower Energy. Journal of Chemical Theory and Computation, 2017, 13, 1219-1228.	2.3	31
67	Stabilization of activated fragments by shellâ€wise construction of an embedding environment. Journal of Computational Chemistry, 2017, 38, 1023-1038.	1.5	11
68	Second-Order Self-Consistent-Field Density-Matrix Renormalization Group. Journal of Chemical Theory and Computation, 2017, 13, 2533-2549.	2.3	60
69	Kooperative Lichtâ€aktivierte Iodâ€•und Photoredoxâ€Katalyse zur Aminierung von Câ€Hâ€Bindungen. Angewandte Chemie, 2017, 129, 8117-8121.	1.6	63
70	Cooperative Lightâ€Activated Iodine and Photoredox Catalysis for the Amination of Câˆ'H Bonds. Angewandte Chemie - International Edition, 2017, 56, 8004-8008.	7.2	181
71	Quantum Chemical Spin Densities for Radical Cations of Photosynthetic Pigment Models. Photochemistry and Photobiology, 2017, 93, 815-833.	1.3	9
72	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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73	Multiconfigurational Effects in Theoretical Resonance Raman Spectra. ChemPhysChem, 2017, 18, 384-393.	1.0	15
74	Context-Driven Exploration of Complex Chemical Reaction Networks. Journal of Chemical Theory and Computation, 2017, 13, 6108-6119.	2.3	87
75	Mechanistic Consequences of Chelate Ligand Stabilization on Nitrogen Fixation by Yandulovâ€"Schrock-Type Complexes. ACS Sustainable Chemistry and Engineering, 2017, 5, 10527-10537.	3.2	8
76	Rigorous Conformational Analysis of Pyrrolidine Enamines with Relevance to Organocatalysis. Helvetica Chimica Acta, 2017, 100, e1700182.	1.0	19
77	Dispersion and Halogen-Bonding Interactions: Binding of the Axial Conformers of Monohalo- and (Â±)-trans-1,2-Dihalocyclohexanes in Enantiopure Alleno-Acetylenic Cages. Journal of the American Chemical Society, 2017, 139, 12190-12200.	6.6	25
78	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
79	Vibrational Density Matrix Renormalization Group. Journal of Chemical Theory and Computation, 2017, 13, 3764-3777.	2.3	46
80	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
81	Sequential Decoupling of Negative-Energy States in Douglasâ€"Krollâ€"Hess Theory. , 2017, , 395-410.		0
82	Self-adaptive tensor network states with multi-site correlators. Journal of Chemical Physics, 2017, 147, 214111.	1.2	11
83	Automated Identification of Relevant Frontier Orbitals for Chemical Compounds and Processes. Chimia, 2017, 71, 170.	0.3	63
84	Error Assessment of Computational Models in Chemistry. Chimia, 2017, 71, 202.	0.3	32
85	Tensor network states with three-site correlators. New Journal of Physics, 2016, 18, 113001.	1.2	3
86	Nitrous Oxide as a Hydrogen Acceptor for the Dehydrogenative Coupling of Alcohols. Angewandte Chemie, 2016, 128, 1886-1890.	1.6	19
87	Real-time feedback from iterative electronic structure calculations. Journal of Computational Chemistry, 2016, 37, 805-812.	1.5	21
88	Nitrous Oxide as a Hydrogen Acceptor for the Dehydrogenative Coupling of Alcohols. Angewandte Chemie - International Edition, 2016, 55, 1854-1858.	7.2	76
89	Calculated Resonance Vibrational Raman Optical Activity Spectra of Naproxen and Ibuprofen. Journal of Physical Chemistry A, 2016, 120, 9740-9748.	1.1	16
90	New methods: general discussion. Faraday Discussions, 2016, 195, 521-556.	1.6	2

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91	Spin-adapted matrix product states and operators. Journal of Chemical Physics, 2016, 144, 134101.	1.2	74
92	<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
93	Systematic Error Estimation for Chemical Reaction Energies. Journal of Chemical Theory and Computation, 2016, 12, 2762-2773.	2.3	71
94	New Approaches for ab initio Calculations of Molecules with Strong Electron Correlation. Chimia, 2016, 70, 244.	0.3	94
95	Accelerating Wave Function Convergence in Interactive Quantum Chemical Reactivity Studies. Journal of Chemical Theory and Computation, 2016, 12, 1228-1235.	2.3	20
96	Molecular Propensity as a Driver for Explorative Reactivity Studies. Journal of Chemical Information and Modeling, 2016, 56, 1470-1478.	2.5	22
97	Uncertainty quantification for quantum chemical models of complex reaction networks. Faraday Discussions, 2016, 195, 497-520.	1.6	64
98	Effect of Chelate Ring Size in Iron(II) Isothiocyanato Complexes with Tetradentate Tripyridyl-alkylamine Ligands on Spin Crossover Properties. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2016, 642, 85-94.	0.6	5
99	Polarizable Embedding Density Matrix Renormalization Group. Journal of Chemical Theory and Computation, 2016, 12, 4242-4253.	2.3	24
100	The Delicate Balance of Static and Dynamic Electron Correlation. Journal of Chemical Theory and Computation, 2016, 12, 3764-3773.	2.3	78
101	A Nonorthogonal State-Interaction Approach for Matrix Product State Wave Functions. Journal of Chemical Theory and Computation, 2016, 12, 5881-5894.	2.3	39
102	Automated Selection of Active Orbital Spaces. Journal of Chemical Theory and Computation, 2016, 12, 1760-1771.	2.3	237
103	An efficient matrix product operator representation of the quantum chemical Hamiltonian. Journal of Chemical Physics, 2015, 143, 244118.	1.2	127
104	Binding of Reactive Oxygen Species at Feï£¿S Cubane Clusters. Chemistry - A European Journal, 2015, 21, 19081-19089.	1.7	7
105	Modeâ€tracking based stationaryâ€point optimization. Journal of Computational Chemistry, 2015, 36, 1429-1438.	1.5	12
106	Special issue on quantum information in chemistry. International Journal of Quantum Chemistry, 2015, 115, 1273-1273.	1.0	2
107	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
108	A stable phosphanyl phosphaketene and its reactivity. Dalton Transactions, 2015, 44, 6431-6438.	1.6	67

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109	Kinetic Consequences of Introducing a Proximal Selenocysteine Ligand into Cytochrome P450cam. Biochemistry, 2015, 54, 6692-6703.	1.2	14
110	Heuristics-Guided Exploration of Reaction Mechanisms. Journal of Chemical Theory and Computation, 2015, 11, 5712-5722.	2.3	127
111	Self-consistent embedding of density-matrix renormalization group wavefunctions in a density functional environment. Journal of Chemical Physics, 2015, 142, 044111.	1.2	34
112	Density matrix renormalization group with efficient dynamical electron correlation through range separation. Journal of Chemical Physics, 2015, 142, 224108.	1.2	86
113	Selection of active spaces for multiconfigurational wavefunctions. Journal of Chemical Physics, 2015, 142, 244104.	1.2	84
114	Relativistic kinetic-balance condition for explicitly correlated basis functions. Journal of Physics B: Atomic, Molecular and Optical Physics, 2015, 48, 245004.	0.6	11
115	Systematic dependence of transitionâ€metal coordination energies on densityâ€functional parametrizations. International Journal of Quantum Chemistry, 2015, 115, 90-98.	1.0	6
116	Sequential Decoupling of Negative-Energy States in Douglasâ€“Krollâ€“Hess Theory. , 2015, , 1-16.		2
117	Determining Factors for the Accuracy of DMRG in Chemistry. Chimia, 2014, 68, 200.	0.3	36
118	Communication: Four-component density matrix renormalization group. Journal of Chemical Physics, 2014, 140, 041101.	1.2	79
119	Activation Barriers of Oxygen Transformation at the Active Site of [FeFe] Hydrogenases. Inorganic Chemistry, 2014, 53, 11890-11902.	1.9	22
120	Gradientâ€driven molecule construction: An inverse approach applied to the design of smallâ€molecule fixating catalysts. International Journal of Quantum Chemistry, 2014, 114, 838-850.	1.0	27
121	Inverse quantum chemistry: Concepts and strategies for rational compound design. International Journal of Quantum Chemistry, 2014, 114, 823-837.	1.0	47
122	Facile Synthesis and Theoretical Conformation Analysis of a Triazineâ€Based Doubleâ€Decker Rotor Molecule with Three Anthracene Blades. Chemistry - A European Journal, 2014, 20, 6934-6938.	1.7	20
123	Electric transition dipole moment in pre-Bornâ€“Oppenheimer molecular structure theory. Journal of Chemical Physics, 2014, 141, 154105.	1.2	3
124	Studying chemical reactivity in a virtual environment. Faraday Discussions, 2014, 169, 89-118.	1.6	37
125	Inaccessibility of the Î¼-hydride species in [FeFe] hydrogenases. Chemical Science, 2014, 5, 215-221.	3.7	48
126	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

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127	Hydrogen-activation mechanism of [Fe] hydrogenase revealed by multi-scale modeling. Chemical Science, 2014, 5, 4474-4482.	3.7	42
128	Interactive Chemical Reactivity Exploration. ChemPhysChem, 2014, 15, 3301-3319.	1.0	47
129	Relativistic Quantum Theory of Many-Electron Systems. Letters in Mathematical Physics, 2014, , 3-29.	0.4	3
130	How Small Amounts of Impurities Are Sufficient to Catalyze the Interconversion of Carbonyl Compounds and Iminium Ions, or Is There a Metathesis through 1,3â€Oxazetidinium Ions? Experiments, Speculations, and Calculations. Helvetica Chimica Acta, 2014, 97, 1177-1203.	1.0	11
131	Quantum entanglement in carbonâ€“carbon, carbonâ€“phosphorus and siliconâ€“silicon bonds. Physical Chemistry Chemical Physics, 2014, 16, 8872-8880.	1.3	39
132	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
133	Editorial. Chimia, 2014, 68, 589.	0.3	0
134	Electric-field effects on the [FeFe]-hydrogenase active site. Chemical Communications, 2013, 49, 8099.	2.2	22
135	Total Synthesis and Detection of the Bilirubin Oxidation Product (Z)-2-(3-Ethenyl-4-methyl-5-oxo-1,5-dihydro-2H-pyrrol-2-ylidene)ethanamide (Z-BOX) Tj ETQq1 1 0.784314 rgBT /Ov	1.4	24
136	Local Spin Analysis and Chemical Bonding. Chemistry - A European Journal, 2013, 19, 15267-15275.	1.7	29
137	Studies toward the Development of New Silicon-Containing Building Blocks for the Direct 18F-Labeling of Peptides. Journal of Medicinal Chemistry, 2013, 56, 7552-7563.	2.9	26
138	Characteristic Raman Optical Activity Signatures of Protein Î²-Sheets. Journal of Physical Chemistry B, 2013, 117, 11943-11953.	1.2	24
139	Predictors for gases of high electrical strength. IEEE Transactions on Dielectrics and Electrical Insulation, 2013, 20, 856-863.	1.8	57
140	Analysis of differences in oxygen sensitivity of Feâ€“S clusters. Dalton Transactions, 2013, 42, 8729.	1.6	31
141	Realâ€time quantum chemistry. International Journal of Quantum Chemistry, 2013, 113, 8-20.	1.0	36
142	Formation of a Ph2PCH(BH3)P(BH3)Ph2 ligand via formal 1,2-borane migration. Chemical Communications, 2013, 49, 1121.	2.2	14
143	Silyl group migration in a P-silylated phosphonium ylide derived from dppm â€" A combined experimental and theoretical study. Inorganic Chemistry Communication, 2013, 32, 28-31.	1.8	6
144	Optimized unrestricted Kohnâ€“Sham potentials from ab initio spin densities. Journal of Chemical Physics, 2013, 138, 044111.	1.2	25

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145	Elimination of the translational kinetic energy contamination in pre-Bornâ€“Oppenheimer calculations. Molecular Physics, 2013, 111, 2086-2092.	0.8	18
146	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
147	Orbital Entanglement in Bond-Formation Processes. Journal of Chemical Theory and Computation, 2013, 9, 2959-2973.	2.3	98
148	An efficient implementation of two-component relativistic exact-decoupling methods for large molecules. Journal of Chemical Physics, 2013, 138, 184105.	1.2	158
149	Theoretical ⁵⁷Fe MÃ¶ssbauer Spectroscopy for Structure Elucidation of [Fe] Hydrogenase Active Site Intermediates. Inorganic Chemistry, 2013, 52, 14205-14215.	1.9	24
150	Kinetic Modeling of Hydrogen Conversion at [Fe] Hydrogenase Active-Site Models. Journal of Physical Chemistry B, 2013, 117, 4806-4817.	1.2	24
151	Toward an Inverse Approach for the Design of Small-Molecule Fixating Catalysts. Materials Research Society Symposia Proceedings, 2013, 1524, 101.	0.1	5
152	Structureâ€“Property Relationships of Fe₄S₄ Clusters. ChemPlusChem, 2013, 78, 1082-1098.	1.3	17
153	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
154	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
155	Spinâ€“Orbit Coupling and Potential Energy Functions of Ar₂⁺ and Kr₂⁺ by High-Resolution Photoelectron Spectroscopy and ab Initio Quantum Chemistry. Journal of Chemical Theory and Computation, 2012, 8, 3671-3685.	2.3	8
156	Spin in densityâ€functional theory. International Journal of Quantum Chemistry, 2012, 112, 3661-3684.	1.0	185
157	Entanglement Measures for Single- and Multireference Correlation Effects. Journal of Physical Chemistry Letters, 2012, 3, 3129-3135.	2.1	143
158	Local relativistic exact decoupling. Journal of Chemical Physics, 2012, 136, 244108.	1.2	88
159	Hydrogen Spillover to Nonreducible Supports. Journal of Physical Chemistry C, 2012, 116, 14274-14283.	1.5	62
160	Relativistic Douglasâ€“Krollâ€“Hess theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 139-149.	6.2	120
161	How Many Chiral Centers Can Raman Optical Activity Spectroscopy Distinguish in a Molecule?. Journal of Physical Chemistry A, 2012, 116, 5410-5419.	1.1	16
162	Accurate ab Initio Spin Densities. Journal of Chemical Theory and Computation, 2012, 8, 1970-1982.	2.3	79

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163	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
164	Hydrogenases and oxygen. Chemical Science, 2012, 3, 1739.	3.7	87
165	Exact decoupling of the relativistic Fock operator. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	238
166	Exact decoupling of the relativistic Fock operator. , 2012, , 205-224.		2
167	New electron correlation theories for transition metal chemistry. Physical Chemistry Chemical Physics, 2011, 13, 6750.	1.3	120
168	Targeting Intermediates of [FeFe]-Hydrogenase by CO and CN Vibrational Signatures. Inorganic Chemistry, 2011, 50, 3888-3900.	1.9	51
169	An enquiry into theoretical bioinorganic chemistry: How heuristic is the character of present-day quantum chemical methods?. Faraday Discussions, 2011, 148, 119-135.	1.6	22
170	Regioselectivity of H Cluster Oxidation. Journal of the American Chemical Society, 2011, 133, 20588-20603.	6.6	47
171	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
172	Quantum-information analysis of electronic states of different molecular structures. Physical Review A, 2011, 83, .	1.0	152
173	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
174	Response to â€œComment on â€˜Accurate frozen-density embedding potentials as a first step towards a subsystem description of covalent bondsâ€™â€•[J. Chem. Phys. 135, 027101 (2011)]. Journal of Chemical Physics, 2011, 135, 027102.	1.2	9
175	Construction of CASCI-type wave functions for very large active spaces. Journal of Chemical Physics, 2011, 134, 224101.	1.2	46
176	Electron Density in Quantum Theory. Structure and Bonding, 2011, , 99-142.	1.0	14
177	MÃ¶ssbauer spectroscopy for heavy elements: a relativistic benchmark study of mercury. Theoretical Chemistry Accounts, 2011, 129, 631-650.	0.5	61
178	Oxygen Coordination to the Active Site of Hmd in Relation to [FeFe] Hydrogenase. European Journal of Inorganic Chemistry, 2011, 2011, 1163-1171.	1.0	18
179	Identifying Protein Î²-Turns with Vibrational Raman Optical Activity. ChemPhysChem, 2011, 12, 1165-1175.	1.0	13
180	Generation of Potential Energy Surfaces in High Dimensions and Their Haptic Exploration. ChemPhysChem, 2011, 12, 3204-3213.	1.0	24

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181	Editorial: Recent Progress in Theoretical and Computational Chemistry. ChemPhysChem, 2011, 12, 3043-3044.	1.0	3
182	Catalytic synthesis of vinylphosphanes via calcium-mediated intermolecular hydrophosphanylation of alkynes and butadiynes. Journal of Organometallic Chemistry, 2011, 696, 216-227.	0.8	42
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