Markus Reiher

List of Publications by Citations

368 papers	19,814 citations	68 h-index	126 g-index
403 ext. papers	22,095 ext. citations	4.9 avg, IF	7.37 L-index

#	Paper	IF	Citations
368	MOLCAS 7: the next generation. *Journal of Computational Chemistry*, **2010**, 31, 224-47	3.5	1425
367	Reparameterization of hybrid functionals based on energy differences of states of different multiplicity. *Theoretical Chemistry Accounts*, **2001**, 107, 48-55	1.9	1115
366	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, **2016**, 37, 506-41	3.5	1047
365	The generalized Douglas–Kroll transformation. *Journal of Chemical Physics*, **2002**, 117, 9215-9226	3.9	558
364	Exact decoupling of the Dirac Hamiltonian. II. The generalized Douglas-Kroll-Hess transformation up to arbitrary order. *Journal of Chemical Physics*, **2004**, 121, 10945-56	3.9	488
363	Assertion and validation of the performance of the B3LYP? functional for the first transition metal row and the G2 test set. *Journal of Chemical Physics*, **2002**, 117, 4729-4737	3.9	463
362	Quantum chemical calculation of vibrational spectra of large molecules--Raman and IR spectra for Buckminsterfullerene. *Journal of Computational Chemistry*, **2002**, 23, 895-910	3.5	445
361	Exact decoupling of the Dirac Hamiltonian. I. General theory. *Journal of Chemical Physics*, **2004**, 121, 2037-47	3.9	406
360	Theoretical study of the Fe(phen)(2)(NCS)(2) spin-crossover complex with reparametrized density functionals. *Inorganic Chemistry*, **2002**, 41, 6928-35	5.1	374
359	OpenMolcas: From Source Code to Insight. *Journal of Chemical Theory and Computation*, **2019**, 15, 5925-5964	5.4	310
358	Elucidating reaction mechanisms on quantum computers. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 7555-7560	11.5	229
357	**2009**,		217
356	Exact decoupling of the relativistic Fock operator. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	183
355	Automated Selection of Active Orbital Spaces. *Journal of Chemical Theory and Computation*, **2016**, 12, 1760-71	6.4	176
354	Douglas–Kroll–Hess Theory: a relativistic electrons-only theory for chemistry. *Theoretical Chemistry Accounts*, **2006**, 116, 241-252	1.9	176
353	Spin in density-functional theory. *International Journal of Quantum Chemistry*, **2012**, 112, 3661-3684	2.1	154
352	Combined spectroscopic and theoretical evidence for a persistent end-on copper superoxo complex. *Angewandte Chemie - International Edition*, **2004**, 43, 4360-3	16.4	150

351	Accurate frozen-density embedding potentials as a first step towards a subsystem description of covalent bonds. *Journal of Chemical Physics*, **2010**, 132, 164101	3.9	149
350	The secret of dimethyl sulfoxide-water mixtures. A quantum chemical study of 1DMSO-nwater clusters. *Journal of the American Chemical Society*, **2002**, 124, 6206-15	16.4	149
349	Cooperative Light-Activated Iodine and Photoredox Catalysis for the Amination of Csp3 -H Bonds. *Angewandte Chemie - International Edition*, **2017**, 56, 8004-8008	16.4	148
348	Density matrix renormalization group calculations on relative energies of transition metal complexes and clusters. *Journal of Chemical Physics*, **2008**, 128, 014104	3.9	147
347	New Benchmark Set of Transition-Metal Coordination Reactions for the Assessment of Density Functionals. *Journal of Chemical Theory and Computation*, **2014**, 10, 3092-103	6.4	142
346	Heavy Grignard reagents: challenges and possibilities of aryl alkaline earth metal compounds. *Chemistry - A European Journal*, **2007**, 13, 6292-306	4.8	137
345	The Density Matrix Renormalization Group Algorithm in Quantum Chemistry. *Zeitschrift Fur Physikalische Chemie*, **2010**, 224, 583-599	3.1	136
344	Quantum-information analysis of electronic states of different molecular structures. *Physical Review A*, **2011**, 83,	2.6	125
343	An efficient implementation of two-component relativistic exact-decoupling methods for large molecules. *Journal of Chemical Physics*, **2013**, 138, 184105	3.9	121
342	Entanglement Measures for Single- and Multireference Correlation Effects. *Journal of Physical Chemistry Letters*, **2012**, 3, 3129-35	6.4	118
341	Comparison of density functionals for differences between the high- (5T2g) and low- (1A1g) spin states of iron(II) compounds. IV. Results for the ferrous complexes [Fe(L)('NHS4')]. *Journal of Chemical Physics*, **2005**, 122, 234321	3.9	118
340	Localizing normal modes in large molecules. *Journal of Chemical Physics*, **2009**, 130, 084106	3.9	117
339	Stable "inverse" sandwich complex with unprecedented organocalcium(I): crystal structures of [(thf)(2)Mg(Br)-C(6)H(2)-2,4,6-Ph(3)] and [(thf)(3)Ca{mu-C(6)H(3)-1,3,5-Ph(3)}Ca(thf)(3)]. *Journal of the American Chemical Society*, **2009**, 131, 2977-85	16.4	117
338	New electron correlation theories for transition metal chemistry. *Physical Chemistry Chemical Physics*, **2011**, 13, 6750-9	3.6	112
337	Modern quantum chemistry with [Open]Molcas. *Journal of Chemical Physics*, **2020**, 152, 214117	3.9	106
336	Intrinsic dinitrogen activation at bare metal atoms. *Angewandte Chemie - International Edition*, **2006**, 45, 6264-88	16.4	105
335	First-principles investigation of the Schrock mechanism of dinitrogen reduction employing the full HIPTN3N ligand. *Inorganic Chemistry*, **2008**, 47, 3634-50	5.1	104
334	Convergence behavior of the density-matrix renormalization group algorithm for optimized orbital orderings. *Journal of Chemical Physics*, **2005**, 122, 024107	3.9	104

333	Estimation of the Vibrational Contribution to the Entropy Change Associated with the Low- to High-Spin Transition in Fe(phen)2(NCS)2 Complexes: Results Obtained by IR and Raman Spectroscopy and DFT Calculations. *Journal of Physical Chemistry A*, **2002**, 106, 12024-12034	2.8	104
332	Heuristics-Guided Exploration of Reaction Mechanisms. *Journal of Chemical Theory and Computation*, **2015**, 11, 5712-22	6.4	102
331	Relativistic Douglas-Kroll-Hess theory. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 139-149	7.9	102
330	An efficient matrix product operator representation of the quantum chemical Hamiltonian. *Journal of Chemical Physics*, **2015**, 143, 244118	3.9	100
329	Basis set and density functional dependence of vibrational Raman optical activity calculations. *Journal of Physical Chemistry A*, **2005**, 109, 7567-74	2.8	95
328	A mode-selective quantum chemical method for tracking molecular vibrations applied to functionalized carbon nanotubes. *Journal of Chemical Physics*, **2003**, 118, 1634-1641	3.9	94
327	Properties of WAu12. *Physical Chemistry Chemical Physics*, **2004**, 6, 11-22	3.6	93
326	Can DFT Accurately Predict Spin Densities? Analysis of Discrepancies in Iron Nitrosyl Complexes. *Journal of Chemical Theory and Computation*, **2011**, 7, 2740-52	6.4	87
325	Theoretical study of catalytic dinitrogen reduction under mild conditions. *Inorganic Chemistry*, **2005**, 44, 9640-2	5.1	87
324	Exploration of Reaction Pathways and Chemical Transformation Networks. *Journal of Physical Chemistry A*, **2019**, 123, 385-399	2.8	85
323	Orbital Entanglement in Bond-Formation Processes. *Journal of Chemical Theory and Computation*, **2013**, 9, 2959-73	6.4	83
322	Calculation of electric-field gradients based on higher-order generalized Douglas-Kroll transformations. *Journal of Chemical Physics*, **2005**, 122, 204107	3.9	80
321	Gas-phase C-H and N-H bond activation by a high valent nitrido-iron dication and NH-transfer to activated olefins. *Journal of the American Chemical Society*, **2008**, 130, 4285-94	16.4	79
320	Hydrogenases and oxygen. *Chemical Science*, **2012**, 3, 1739	9.4	78
319	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	2.8	78
318	Comparative analysis of local spin definitions. *Journal of Chemical Physics*, **2005**, 122, 34102	3.9	77
317	Density matrix renormalization group with efficient dynamical electron correlation through range separation. *Journal of Chemical Physics*, **2015**, 142, 224108	3.9	74
316	Exact decoupling of the Dirac Hamiltonian. III. Molecular properties. *Journal of Chemical Physics*, **2006**, 124, 64102	3.9	74

315	New Approaches for ab initio Calculations of Molecules with Strong Electron Correlation. *Chimia*, **2016**, 70, 244-51	1.3	74
314	Multireference Perturbation Theory with Cholesky Decomposition for the Density Matrix Renormalization Group. *Journal of Chemical Theory and Computation*, **2017**, 13, 451-459	6.4	73
313	Selection of active spaces for multiconfigurational wavefunctions. *Journal of Chemical Physics*, **2015** , 142, 244104	3.9	73
312	Decomposition of density matrix renormalization group states into a Slater determinant basis. *Journal of Chemical Physics*, **2007**, 126, 244109	3.9	73
311	Binding N2, N2H2, N2H4, and NH3 to transition-metal sulfur sites: modeling potential intermediates of biological N2 fixation. *Chemistry - A European Journal*, **2004**, 10, 819-30	4.8	73
310	The density matrix renormalization group in chemistry and molecular physics: Recent developments and new challenges. *Journal of Chemical Physics*, **2020**, 152, 040903	3.9	71
309	Capture and characterization of a reactive haem□carbenoid complex in an artificial metalloenzyme. *Nature Catalysis*, **2018**, 1, 578-584	36.5	71
308	Accurate ab Initio Spin Densities. *Journal of Chemical Theory and Computation*, **2012**, 8, 1970-1982	6.4	70
307	Complete-graph tensor network states: a new fermionic wave function ansatz for molecules. *New Journal of Physics*, **2010**, 12, 103008	2.9	70
306	Tetracycline and derivatives□ssignment of IR and Raman spectra via DFT calculations. *Physical Chemistry Chemical Physics*, **2003**, 5, 1149-1157	3.6	70
305	Can Raman optical activity separate axial from local chirality? A theoretical study of helical deca-alanine. *ChemPhysChem*, **2006**, 7, 2189-96	3.2	69
304	Engineering Molecular Iodine Catalysis for Alkyl□Nitrogen Bond Formation. *ACS Catalysis*, **2018**, 8, 3918-3925	13.1	68
303	Local relativistic exact decoupling. *Journal of Chemical Physics*, **2012**, 136, 244108	3.9	68
302	Formation of a nickel-methyl species in methyl-coenzyme m reductase, an enzyme catalyzing methane formation. *Journal of the American Chemical Society*, **2007**, 129, 11028-9	16.4	68
301	Chirality-induced switch in hydrogen-bond topology: tetrameric methyl lactate clusters in the gas phase. *Angewandte Chemie - International Edition*, **2006**, 45, 3440-5	16.4	68
300	Theoretical Raman optical activity study of the beta domain of rat metallothionein. *Journal of Physical Chemistry B*, **2010**, 114, 1057-63	3.4	67
299	The Matter Simulation (R)evolution. *ACS Central Science*, **2018**, 4, 144-152	16.8	66
298	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, 6558-73	3.4	66

297	On the definition of local spin in relativistic and nonrelativistic quantum chemistry. *Faraday Discussions*, **2007**, 135, 97-124; discussion 125-49, 503-6	3.6	66
296	Nitrogen fixation under mild ambient conditions: part I--the initial dissociation/association step at molybdenum triamidoamine complexes. *Chemistry - A European Journal*, **2005**, 11, 7448-60	4.8	66
295	Understanding the signatures of secondary-structure elements in proteins with Raman optical activity spectroscopy. *Chemistry - A European Journal*, **2009**, 15, 13491-508	4.8	65
294	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, 10907-20	16.4	64
293	Stoichiometric Reactions of Enamines Derived from Diphenylprolinol Silyl Ethers with Nitro Olefins and Lessons for the Corresponding Organocatalytic Conversions a Survey. *Helvetica Chimica Acta*, **2013**, 96, 799-852	2	63
292	Isoelectronic Arduengo-Type Carbene Analogues with the Group IIIa Elements Boron, Aluminum, Gallium, and Indium **1998**, 1998, 305-310		62
291	Analysis of electron density distributions from subsystem density functional theory applied to coordination bonds. *Chemical Physics Letters*, **2008**, 461, 353-359	2.5	62
290	Systematic Error Estimation for Chemical Reaction Energies. *Journal of Chemical Theory and Computation*, **2016**, 12, 2762-73	6.4	61
289	A stable phosphanyl phosphaketene and its reactivity. *Dalton Transactions*, **2015**, 44, 6431-8	4.3	60
288	Communication: four-component density matrix renormalization group. *Journal of Chemical Physics*, **2014**, 140, 041101	3.9	60
287	Analytic high-order Douglas-Kroll-Hess electric field gradients. *Journal of Chemical Physics*, **2007**, 127, 074105	3.9	60
286	Trinuclear copper(II) complexes derived from Schiff-base ligands based on a 6-amino-6-deoxyglucopyranoside: structural and magnetic characterization. *Inorganic Chemistry*, **2006**, 45, 10066-76	5.1	60
285	The Delicate Balance of Static and Dynamic Electron Correlation. *Journal of Chemical Theory and Computation*, **2016**, 12, 3764-73	6.4	59
284	Raman optical activity spectra of chiral transition metal complexes. *Chemical Physics*, **2008**, 346, 212-223	2.3	59
283	Spektroskopischer und theoretischer Nachweis eines best digen End-on-Kupfersuperoxokomplexes. *Angewandte Chemie*, **2004**, 116, 4460-4464	3.6	59
282	Relativistic DMRG calculations on the curve crossing of cesium hydride. *Journal of Chemical Physics*, **2005**, 123, 184105	3.9	58
281	M ssbauer spectroscopy for heavy elements: a relativistic benchmark study of mercury. *Theoretical Chemistry Accounts*, **2011**, 129, 631-650	1.9	57
280	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	3.9	57

279	Finding a needle in a haystack: direct determination of vibrational signatures in complex systems. *New Journal of Chemistry*, **2007**, 31, 818	3.6	57
278	Relativistic Effects on the Topology of the Electron Density. *Journal of Chemical Theory and Computation*, **2007**, 3, 2182-97	6.4	57
277	Synthesis of chiral self-assembling rhombs and their characterization in solution, in the gas phase, and at the liquid-solid interface. *Journal of the American Chemical Society*, **2005**, 127, 17672-85	16.4	56
276	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, 64103	3.9	55
275	Quantum Chemical Calculation of Raman Intensities for Large Molecules: The Photoisomerization of [{Fe(PR3)}2(N2H2)] (= 1,2-bis(2-Mercaptophenylthio)-Ethane(2-)). *Zeitschrift Fur Physikalische Chemie*, **2003**, 217, 91-104	3.1	55
274	Nitrous Oxide as a Hydrogen Acceptor for the Dehydrogenative Coupling of Alcohols. *Angewandte Chemie - International Edition*, **2016**, 55, 1854-8	16.4	55
273	A Theoretical Challenge: Transition-Metal Compounds. *Chimia*, **2009**, 63, 140-145	1.3	54
272	Ligands for dinitrogen fixation at Schrock-type catalysts. *Inorganic Chemistry*, **2009**, 48, 1638-48	5.1	54
271	Fluorescence kinetics of aqueous solutions of tetracycline and its complexes with Mg2+ and Ca2+. *Photochemical and Photobiological Sciences*, **2003**, 2, 1107-17	4.2	54
270	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	1.9	54
269	Kooperative Licht-aktivierte Iod- und Photoredox-Katalyse zur Aminierung von C -H-Bindungen. *Angewandte Chemie*, **2017**, 129, 8117-8121	3.6	53
268	Automated Identification of Relevant Frontier Orbitals for Chemical Compounds and Processes. *Chimia*, **2017**, 71, 170-176	1.3	53
267	Two-Component Relativistic Calculations of Electric-Field Gradients Using Exact Decoupling Methods: Spin-orbit and Picture-Change Effects. *Journal of Chemical Theory and Computation*, **2012**, 8, 4239-48	6.4	53
266	First-Principles Approach to Vibrational Spectroscopy of Biomolecules **2006**, 85-132		52
265	Spin-adapted matrix product states and operators. *Journal of Chemical Physics*, **2016**, 144, 134101	3.9	51
264	Error-Controlled Exploration of Chemical Reaction Networks with Gaussian Processes. *Journal of Chemical Theory and Computation*, **2018**, 14, 5238-5248	6.4	51
263	M(O)V(I)P(AC): vibrational spectroscopy with a robust meta-program for massively parallel standard and inverse calculations. *Journal of Computational Chemistry*, **2012**, 33, 2186-98	3.5	50
262	Enhancement and de-enhancement effects in vibrational resonance Raman optical activity. *Journal of Chemical Physics*, **2010**, 132, 044113	3.9	50

261	The first photoexcitation step of ruthenium-based models for artificial photosynthesis highlighted by resonance Raman spectroscopy. *Journal of Physical Chemistry B*, **2007**, 111, 6078-87	3.4	50
260	Spin states in polynuclear clusters: the [Fe2O2] core of the methane monooxygenase active site. *Journal of Computational Chemistry*, **2006**, 27, 1223-39	3.5	50
259	Dinuclear diazene iron and ruthenium complexes as models for studying nitrogenase activity. *Chemistry - A European Journal*, **2001**, 7, 5195-202	4.8	50
258	Context-Driven Exploration of Complex Chemical Reaction Networks. *Journal of Chemical Theory and Computation*, **2017**, 13, 6108-6119	6.4	49
257	Orbital entanglement and CASSCF analysis of the Ru-NO bond in a Ruthenium nitrosyl complex. *Physical Chemistry Chemical Physics*, **2015**, 17, 14383-92	3.6	49
256	Theoretical study of dioxygen induced inhibition of [FeFe]-hydrogenase. *Inorganic Chemistry*, **2009**, 48, 7127-40	5.1	49
255	Calculation of Ligand Dissociation Energies in Large Transition-Metal Complexes. *Journal of Chemical Theory and Computation*, **2018**, 14, 2456-2468	6.4	48
254	Targeting intermediates of [FeFe]-hydrogenase by CO and CN vibrational signatures. *Inorganic Chemistry*, **2011**, 50, 3888-900	5.1	48
253	A stable six-coordinate intermediate in ammonia-dinitrogen exchange at Schrock's molybdenum catalyst. *Chemistry - A European Journal*, **2009**, 15, 5073-82	4.8	48
252	Topological analysis of electron densities from Kohn-Sham and subsystem density functional theory. *Journal of Chemical Physics*, **2008**, 128, 044114	3.9	48
251	THF solvates of extremely soluble bis(2,4,6-trimethylphenyl)calcium and tris(2,6-dimethoxyphenyl)dicalcium iodide. *Angewandte Chemie - International Edition*, **2007**, 46, 1618-23	16.4	48
250	Calculated Raman optical activity signatures of tryptophan side chains. *ChemPhysChem*, **2008**, 9, 2177-80	3.2	48
249	Construction of environment states in quantum-chemical density-matrix renormalization group calculations. *Journal of Chemical Physics*, **2006**, 124, 034103	3.9	47
248	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, 873-84	3.7	47
247	Uncertainty quantification for quantum chemical models of complex reaction networks. *Faraday Discussions*, **2016**, 195, 497-520	3.6	47
246	Second-Order Self-Consistent-Field Density-Matrix Renormalization Group. *Journal of Chemical Theory and Computation*, **2017**, 13, 2533-2549	6.4	46
245	The Exploration of Chemical Reaction Networks. *Annual Review of Physical Chemistry*, **2020**, 71, 121-142	15.7	46
244	From rare gas atoms to fullerenes: spherical aromaticity studied from the point of view of atomic structure theory. *Chemistry - A European Journal*, **2003**, 9, 5442-52	4.8	46

243	Hydrogen Spillover to Nonreducible Supports. *Journal of Physical Chemistry C*, **2012**, 116, 14274-14283	3.8	45
242	Subvalent Organometallic Compounds of the Alkaline Earth Metals in Low Oxidation States. *European Journal of Inorganic Chemistry*, **2010**, 2010, 197-216	2.3	45
241	Relevance of the electric-dipole--electric-quadrupole contribution to Raman optical activity spectra. *Journal of Physical Chemistry B*, **2008**, 112, 2218-32	3.4	45
240	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, 10078-87	4.8	45
239	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, 10649-60	3.4	44
238	Calculated Raman optical activity spectra of 1,6-anhydro-beta-D-glucopyranose. *Journal of Physical Chemistry A*, **2009**, 113, 8268-77	2.8	44
237	On the emergence of molecular structure. *Physical Review A*, **2011**, 83,	2.6	44
236	Inaccessibility of the hydride species in [FeFe] hydrogenases. *Chemical Science*, **2014**, 5, 215-221	9.4	43
235	Inverse quantum chemistry: Concepts and strategies for rational compound design. *International Journal of Quantum Chemistry*, **2014**, 114, 823-837	2.1	42
234	Construction of CASCI-type wave functions for very large active spaces. *Journal of Chemical Physics*, **2011**, 134, 224101	3.9	42
233	Regioselectivity of H cluster oxidation. *Journal of the American Chemical Society*, **2011**, 133, 20588-603	16.4	42
232	The Douglas Kroll Hess electron density at an atomic nucleus. *Chemical Physics Letters*, **2008**, 465, 157-164	2.5	42
231	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	2.8	41
230	Organofluorosilanes as model compounds for 18F-labeled silicon-based PET tracers and their hydrolytic stability: experimental data and theoretical calculations (PET = positron emission tomography). *Chemistry - A European Journal*, **2009**, 15, 3736-43	4.8	41
229	autoCAS: A Program for Fully Automated Multiconfigurational Calculations. *Journal of Computational Chemistry*, **2019**, 40, 2216-2226	3.5	40
228	Unravelling the quantum-entanglement effect of noble gas coordination on the spin ground state of CUO. *Physical Chemistry Chemical Physics*, **2014**, 16, 719-27	3.6	40
227	A photochemical activation scheme of inert dinitrogen by dinuclear Ru(II) and Fe(II) complexes. *Chemistry - A European Journal*, **2004**, 10, 4443-53	4.8	40
226	Correlated ab initio calculations of spectroscopic parameters of SnO within the framework of the higher-order generalized Douglas-Kroll transformation. *Journal of Chemical Physics*, **2004**, 120, 8624-31	3.9	40

225	Large-Scale Quantum Dynamics with Matrix Product States. *Journal of Chemical Theory and Computation*, **2019**, 15, 3481-3498	6.4	39
224	Analysis of the Cartesian Tensor Transfer Method for Calculating Vibrational Spectra of Polypeptides. *Journal of Chemical Theory and Computation*, **2011**, 7, 1867-81	6.4	39
223	Predictors for gases of high electrical strength. *IEEE Transactions on Dielectrics and Electrical Insulation*, **2013**, 20, 856-863	2.3	38
222	The Shell Structure of Atoms. *Journal of Chemical Theory and Computation*, **2008**, 4, 286-96	6.4	38
221	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	2.3	38
220	Convergence characteristics and efficiency of mode-tracking calculations on pre-selected molecular vibrations. *Physical Chemistry Chemical Physics*, **2004**, 6, 4621	3.6	38
219	Hydrogen-activation mechanism of [Fe] hydrogenase revealed by multi-scale modeling. *Chemical Science*, **2014**, 5, 4474-4482	9.4	37
218	A unifying structural and electronic concept for Hmd and [FeFe] hydrogenase active sites. *Inorganic Chemistry*, **2010**, 49, 5818-23	5.1	37
217	Intensity-carrying modes in Raman and Raman optical activity spectroscopy. *ChemPhysChem*, **2009**, 10, 2049-57	3.2	37
216	Coupled-cluster Raman intensities: Assessment and comparison with multiconfiguration and density functional methods. *Journal of Chemical Physics*, **2002**, 117, 8623-8633	3.9	37
215	Reliable Estimation of Prediction Uncertainty for Physicochemical Property Models. *Journal of Chemical Theory and Computation*, **2017**, 13, 3297-3317	6.4	36
214	Extracting elements of molecular structure from the all-particle wave function. *Journal of Chemical Physics*, **2011**, 135, 204302	3.9	36
213	Nuclear quadrupole moment of 119Sn. *Journal of Physical Chemistry A*, **2008**, 112, 1666-72	2.8	36
212	Interactive chemical reactivity exploration. *ChemPhysChem*, **2014**, 15, 3301-19	3.2	35
211	Quantum entanglement in carbon-carbon, carbon-phosphorus and silicon-silicon bonds. *Physical Chemistry Chemical Physics*, **2014**, 16, 8872-80	3.6	35
210	Intensity tracking for theoretical infrared spectroscopy of large molecules. *Journal of Chemical Physics*, **2009**, 130, 064105	3.9	35
209	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	16.4	34
208	Selective calculation of high-intensity vibrations in molecular resonance Raman spectra. *Journal of Chemical Physics*, **2008**, 129, 204103	3.9	34

207	Spin□Spin interactions in polynuclear transition-metal complexes. *Chemical Physics Letters*, **2008**, 451, 301-308	2.5	34
206	Metal thiolate complexes binding molecular nitrogen under mild conditions: [□N2{Ru(PiPr3)(N2Me2S2)}2], the first dinuclear example. *Inorganica Chimica Acta*, **2003**, 348, 194-198	2.7	34
205	Catalytic synthesis of vinylphosphanes via calcium-mediated intermolecular hydrophosphanylation of alkynes and butadiynes. *Journal of Organometallic Chemistry*, **2011**, 696, 216-227	2.3	33
204	**2014**,		32
203	Intrinsische Stickstoff-Aktivierung an □backten□ Metallatomen. *Angewandte Chemie*, **2006**, 118, 6412-6437	3.6	32
202	A quantum-chemical study of dinitrogen reduction at mononuclear iron-sulfur complexes with hints to the mechanism of nitrogenase. *Chemistry - A European Journal*, **2002**, 8, 5332-9	4.8	32
201	Measuring multi-configurational character by orbital entanglement. *Molecular Physics*, **2017**, 115, 2110-2119	2.1	31
200	Vibrational Density Matrix Renormalization Group. *Journal of Chemical Theory and Computation*, **2017**, 13, 3764-3777	6.4	31
199	Importance of backbone angles versus amino acid configurations in peptide vibrational Raman optical activity spectra. *Chemical Physics*, **2008**, 343, 200-209	2.3	31
198	Determining factors for the accuracy of DMRG in chemistry. *Chimia*, **2014**, 68, 200-3	1.3	30
197	Self-consistent embedding of density-matrix renormalization group wavefunctions in a density functional environment. *Journal of Chemical Physics*, **2015**, 142, 044111	3.9	29
196	Mode Tracking of Preselected Vibrations of One-Dimensional Molecular Wires. *Journal of Physical Chemistry A*, **2004**, 108, 2053-2061	2.8	29
195	Semiempirical molecular orbital models based on the neglect of diatomic differential overlap approximation. *International Journal of Quantum Chemistry*, **2018**, 118, e25799	2.1	29
194	Systematic microsolvation approach with a cluster-continuum scheme and conformational sampling. *Journal of Computational Chemistry*, **2020**, 41, 1144-1155	3.5	28
193	Car-Parrinello molecular dynamics study of the initial dinitrogen reduction step in Sellmann-type nitrogenase model complexes. *Chemistry - A European Journal*, **2005**, 11, 574-83	4.8	28
192	Local spin analysis and chemical bonding. *Chemistry - A European Journal*, **2013**, 19, 15267-75	4.8	27
191	Real-time quantum chemistry. *International Journal of Quantum Chemistry*, **2013**, 113, 8-20	2.1	27
190	Basis set representation of the electron density at an atomic nucleus. *Journal of Chemical Physics*, **2010**, 133, 144111	3.9	27

189	A Nonorthogonal State-Interaction Approach for Matrix Product State Wave Functions. *Journal of Chemical Theory and Computation*, **2016**, 12, 5881-5894	6.4	26
188	Studying chemical reactivity in a virtual environment. *Faraday Discussions*, **2014**, 169, 89-118	3.6	26
187	Theoretical study on the spin-state energy splittings and local spin in cationic [Re]-Cn-[Re] complexes. *Inorganic Chemistry*, **2005**, 44, 6174-82	5.1	26
186	Gaussian Process-Based Refinement of Dispersion Corrections. *Journal of Chemical Theory and Computation*, **2019**, 15, 6046-6060	6.4	25
185	Prediction of Raman optical activity spectra of chiral 3-acetylcamphorato-cobalt complexes. *ChemPhysChem*, **2010**, 11, 1876-87	3.2	25
184	Two-component methods and the generalised Douglas□Kroll transformation. *Theoretical and Computational Chemistry*, **2002**, 11, 622-663		25
183	Studies toward the development of new silicon-containing building blocks for the direct (18)F-labeling of peptides. *Journal of Medicinal Chemistry*, **2013**, 56, 7552-63	8.3	24
182	Gradient-driven molecule construction: An inverse approach applied to the design of small-molecule fixating catalysts. *International Journal of Quantum Chemistry*, **2014**, 114, 838-850	2.1	24
181	Error Assessment of Computational Models in Chemistry. *Chimia*, **2017**, 71, 202-208	1.3	23
180	Characteristic Raman optical activity signatures of protein □sheets. *Journal of Physical Chemistry B*, **2013**, 117, 11943-53	3.4	23
179	Haptic quantum chemistry. *Journal of Computational Chemistry*, **2009**, 30, 2010-20	3.5	23
178	Restrained optimization of broken-symmetry determinants. *International Journal of Quantum Chemistry*, **2009**, 109, 2430-2446	2.1	23
177	On the R-dependence of the spin-orbit coupling constant: Potential energy functions of Xe(2) (+) by high-resolution photoelectron spectroscopy and ab initio quantum chemistry. *Journal of Chemical Physics*, **2008**, 128, 234306	3.9	23
176	THF-Komplexe von extrem l□lichem Bis(2,4,6-trimethylphenyl)calcium und Tris(2,6-dimethoxyphenyl)dicalciumiodid. *Angewandte Chemie*, **2007**, 119, 1642-1647	3.6	23
175	Vibrational center-ligand couplings in transition metal complexes. *Journal of Computational Chemistry*, **2004**, 25, 587-97	3.5	23
174	Analysis of differences in oxygen sensitivity of Fe-S clusters. *Dalton Transactions*, **2013**, 42, 8729-35	4.3	22
173	Dispersion and Halogen-Bonding Interactions: Binding of the Axial Conformers of Monohalo- and (□)-trans-1,2-Dihalocyclohexanes in Enantiopure Alleno-Acetylenic Cages. *Journal of the American Chemical Society*, **2017**, 139, 12190-12200	16.4	22
172	Kinetic modeling of hydrogen conversion at [Fe] hydrogenase active-site models. *Journal of Physical Chemistry B*, **2013**, 117, 4806-17	3.4	22

171	DMRG control using an automated Richardson-type error protocol. *Molecular Physics*, **2010**, 108, 501-512	1.7	22
170	An enquiry into theoretical bioinorganic chemistry: how heuristic is the character of present-day quantum chemical methods?. *Faraday Discussions*, **2011**, 148, 119-35; discussion 207-28	3.6	22
169	Electromagnetic fields in relativistic one-particle equations. *Chemical Physics*, **2009**, 356, 205-218	2.3	22
168	Chirality-Induced Switch in Hydrogen-Bond Topology: Tetrameric Methyl Lactate Clusters in the Gas Phase. *Angewandte Chemie*, **2006**, 118, 3518-3523	3.6	22
167	TRANSGRESSING THEORY BOUNDARIES: THE GENERALIZED DOUGLAS□KROLL TRANSFORMATION. *Recent Advances in Computational*, **2004**, 137-190		22
166	Theoretical 57Fe M□ssbauer spectroscopy for structure elucidation of [Fe] hydrogenase active site intermediates. *Inorganic Chemistry*, **2013**, 52, 14205-15	5.1	21
165	Generation of potential energy surfaces in high dimensions and their haptic exploration. *ChemPhysChem*, **2011**, 12, 3204-13	3.2	21
164	Do Divalent [{HC(CR?NR??)2}E] Compounds Contain E(I) or E(III) (E = B, Al, Ga, In)? On the Correspondence of Formal Oxidation Numbers, Lewis Structures, and Reactivity. *European Journal of Inorganic Chemistry*, **2002**, 2002, 1854-1863	2.3	21
163	Optimization of highly excited matrix product states with an application to vibrational spectroscopy. *Journal of Chemical Physics*, **2019**, 150, 094113	3.9	20
162	Polarizable Embedding Density Matrix Renormalization Group. *Journal of Chemical Theory and Computation*, **2016**, 12, 4242-53	6.4	20
161	Activation barriers of oxygen transformation at the active site of [FeFe] hydrogenases. *Inorganic Chemistry*, **2014**, 53, 11890-902	5.1	20
160	Analysis of vibrational Raman optical activity signatures of the (TG)(N) and (GG)(N) conformations of isotactic polypropylene chains in terms of localized modes. *Journal of Physical Chemistry A*, **2010**, 114, 7198-212	2.8	20
159	Regular no-pair Dirac operators: Numerical study of the convergence of high-order Douglas□Kroll□Hess transformations. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2007**, 360, 603-607	2.3	20
158	QM/MM vibrational mode tracking. *Journal of Computational Chemistry*, **2008**, 29, 2460-70	3.5	20
157	(N,N) vs. (N,S) chelation of palladium in asymmetric allylic substitution using bis(thiazoline) ligands: A theoretical and experimental study. *Journal of Organometallic Chemistry*, **2008**, 693, 2499-2508	2.3	20
156	Binding H2, N2, H-, and BH3 to transition-metal sulfur sites: synthesis and properties of [RuL(PR3)(N2Me2S2)] Complexes (L=eta2-H2, H-, BH3; R=Cy, iPr). *Chemistry - A European Journal*, **2004**, 10, 4214-24	4.8	20
155	A Wavefunction-Based Criterion for the Detection of Intermolecular Interactions in Molecular Dynamics Simulations. *Journal of Physical Chemistry A*, **2003**, 107, 4141-4146	2.8	20
154	Steering Orbital Optimization out of Local Minima and Saddle Points Toward Lower Energy. *Journal of Chemical Theory and Computation*, **2017**, 13, 1219-1228	6.4	19

153	Hardware efficient quantum algorithms for vibrational structure calculations. *Chemical Science*, **2020**, 11, 6842-6855	9.4	19
152	Redox-Active Chiroptical Switching in Mono- and Bis-Iron Ethynylcarbo[6]helicenes Studied by Electronic and Vibrational Circular Dichroism and Resonance Raman Optical Activity. *Chemistry - A European Journal*, **2018**, 24, 15067-15079	4.8	19
151	Electric-field effects on the [FeFe]-hydrogenase active site. *Chemical Communications*, **2013**, 49, 8099-105	4.8	19
150	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 A). *Organic Letters*, **2013**, 15, 4608-11	6.2	19
149	Optimized unrestricted Kohn-Sham potentials from ab initio spin densities. *Journal of Chemical Physics*, **2013**, 138, 044111	3.9	19
148	Bonding Properties of Amidinate Complexes of the Group 14 Elements Silicon, Germanium, Tin, and Lead in Their Divalent and Tetravalent Oxidation States *Inorganic Chemistry*, **1999**, 38, 29-37	5.1	19
147	Self-Parametrizing System-Focused Atomistic Models. *Journal of Chemical Theory and Computation*, **2020**, 16, 1646-1665	6.4	18
146	Statistical Analysis of Semiclassical Dispersion Corrections. *Journal of Chemical Theory and Computation*, **2018**, 14, 2480-2494	6.4	18
145	Oxygen Coordination to the Active Site of Hmd in Relation to [FeFe] Hydrogenase. *European Journal of Inorganic Chemistry*, **2011**, 2011, 1163-1171	2.3	18
144	Rigorous Conformational Analysis of Pyrrolidine Enamines with Relevance to Organocatalysis. *Helvetica Chimica Acta*, **2017**, 100, e1700182	2	17
143	Direct targeting of adsorbate vibrations with mode-tracking. *Surface Science*, **2006**, 600, 1891-1900	1.8	17
142	Nitrous Oxide as a Hydrogen Acceptor for the Dehydrogenative Coupling of Alcohols. *Angewandte Chemie*, **2016**, 128, 1886-1890	3.6	17
141	Molecular Propensity as a Driver for Explorative Reactivity Studies. *Journal of Chemical Information and Modeling*, **2016**, 56, 1470-8	6.1	17
140	Quantum computing enhanced computational catalysis. *Physical Review Research*, **2021**, 3,	3.9	17
139	Relativistic effects on the Fukui function. *Theoretical Chemistry Accounts*, **2010**, 127, 195-202	1.9	16
138	Sigma-donor and pi-acceptor stacking interactions in a trans-2-linked C60-cobalt(II) tetraphenylporphyrin diad. *Angewandte Chemie - International Edition*, **2006**, 45, 3368-72	16.4	16
137	Real-time feedback from iterative electronic structure calculations. *Journal of Computational Chemistry*, **2016**, 37, 805-12	3.5	16
136	Quantum system partitioning at the single-particle level. *Journal of Chemical Physics*, **2018**, 149, 184104	3.9	16

135	Facile synthesis and theoretical conformation analysis of a triazine-based double-decker rotor molecule with three anthracene blades. *Chemistry - A European Journal*, **2014**, 20, 6934-8	4.8	15
134	Structure-Property Relationships of Fe S Clusters. *ChemPlusChem*, **2013**, 78, 1082-1098	2.8	15
133	Syntheses of N-(Diphenylphosphanyl)-2-pyridylmethylamine and Its Use as a Ligand in Magnesium and Zinc Complexes. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2007**, 633, 893-902	1.3	15
132	Numerical electronic structure calculations for atoms. II. Generalized variable transformation and relativistic calculations. *International Journal of Quantum Chemistry*, **2000**, 76, 473-499	2.1	15
131	Experimental Evidence for the Existence of Neutral P6: A New Allotrope of Phosphorus. *Angewandte Chemie - International Edition*, **1999**, 38, 3513-3515	16.4	15
130	The electrostatic potential as a descriptor for the protonation propensity in automated exploration of reaction mechanisms. *Faraday Discussions*, **2019**, 220, 443-463	3.6	14
129	A Systems Theory for Chemistry. *Foundations of Chemistry*, **2003**, 5, 23-41	0.7	14
128	QUANTUM CHEMICAL INVESTIGATIONS INTO THE PROBLEM OF BIOLOGICAL NITROGEN FIXATION: SELLMANN-TYPE METALSULFUR MODEL COMPLEXES. *Advances in Inorganic Chemistry*, **2004**, 55-100	2.1	14
127	A comparative study of finite nucleus models for low-lying states of few-electron high-Z atoms. *Chemical Physics Letters*, **2000**, 320, 457-468	2.5	14
126	Calculated Resonance Vibrational Raman Optical Activity Spectra of Naproxen and Ibuprofen. *Journal of Physical Chemistry A*, **2016**, 120, 9740-9748	2.8	14
125	Accelerating Wave Function Convergence in Interactive Quantum Chemical Reactivity Studies. *Journal of Chemical Theory and Computation*, **2016**, 12, 1228-35	6.4	14
124	Kinetic consequences of introducing a proximal selenocysteine ligand into cytochrome P450cam. *Biochemistry*, **2015**, 54, 6692-703	3.2	13
123	Generalized Pauli constraints in small atoms. *Physical Review A*, **2018**, 97,	2.6	13
122	Elimination of the translational kinetic energy contamination in pre-BornOppenheimer calculations. *Molecular Physics*, **2013**, 111, 2086-2092	1.7	13
121	Identifying protein turns with vibrational Raman optical activity. *ChemPhysChem*, **2011**, 12, 1165-75	3.2	13
120	Intensity Tracking for Vibrational Spectra of Large Molecules. *Chimia*, **2009**, 63, 270-274	1.3	13
119	Ion dynamics in confined spaces: sodium ion mobility in icosahedral container molecules. *Angewandte Chemie - International Edition*, **2010**, 49, 7465-9	16.4	13
118	Understanding the template preorganization step of an artificial arginine receptor. *Journal of the American Chemical Society*, **2005**, 127, 8748-56	16.4	13

117	Self-consistent treatment of the frequency-independent Breit interaction in Dirac-Fock and MCSCF calculations of atomic structures: I. Theoretical considerations. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1999**, 32, 5489-5505	1.3	13
116	Molassembler: Molecular Graph Construction, Modification, and Conformer Generation for Inorganic and Organic Molecules. *Journal of Chemical Information and Modeling*, **2020**, 60, 3884-3900	6.1	12
115	Formation of a Ph2PCH(BH3)P(BH3)Ph2 ligand via formal 1,2-borane migration. *Chemical Communications*, **2013**, 49, 1121-3	5.8	12
114	The "invisible" 13C NMR chemical shift of the central carbon atom in [(Ph3PAu)6C]2+: a theoretical investigation. *Chemistry - A European Journal*, **2005**, 11, 1677-86	4.8	12
113	Mechanism Deduction from Noisy Chemical Reaction Networks. *Journal of Chemical Theory and Computation*, **2019**, 15, 357-370	6.4	12
112	Comprehensive Analysis of the Neglect of Diatomic Differential Overlap Approximation. *Journal of Chemical Theory and Computation*, **2018**, 14, 5169-5179	6.4	12
111	Multiconfigurational Effects in Theoretical Resonance Raman Spectra. *ChemPhysChem*, **2017**, 18, 384-393	3.2	11
110	Minimum Energy Paths and Transition States by Curve Optimization. *Journal of Chemical Theory and Computation*, **2018**, 14, 3091-3099	6.4	11
109	Self-adaptive tensor network states with multi-site correlators. *Journal of Chemical Physics*, **2017**, 147, 214111	3.9	11
108	Mode-tracking based stationary-point optimization. *Journal of Computational Chemistry*, **2015**, 36, 1429-38	3.5	11
107	Spin Interactions in Cluster Chemistry. *Advances in Inorganic Chemistry*, **2010**, 177-230	2.1	11
106	A C2v-symmetric barbaralane. *Angewandte Chemie - International Edition*, **2002**, 41, 3429-33	16.4	11
105	A quantum chemical study on the stability of [3n]-allenophanes (n=2-4). *Physical Chemistry Chemical Physics*, **2000**, 2, 2205-2210	3.6	11
104	Generalized elimination of the global translation from explicitly correlated Gaussian functions. *Journal of Chemical Physics*, **2018**, 148, 084112	3.9	10
103	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	6.4	10
102	How many chiral centers can Raman optical activity spectroscopy distinguish in a molecule?. *Journal of Physical Chemistry A*, **2012**, 116, 5410-9	2.8	10
101	Synthesis, Structures, and Magnetic Properties of N-Trialkylsilyl-8-amidoquinoline Complexes of Chromium, Manganese, Iron, and Cobalt as well as of Wheel-Like Hexanuclear Iron(II) and Manganese(II) Bis(8-amidoquinoline). *European Journal of Inorganic Chemistry*, **2010**, 2010, 1777-1790	2.3	10
100	Stabilization of activated fragments by shell-wise construction of an embedding environment. *Journal of Computational Chemistry*, **2017**, 38, 1023-1038	3.5	9

99	How Small Amounts of Impurities Are Sufficient to Catalyze the Interconversion of Carbonyl Compounds and Iminium Ions, or Is There a Metathesis through 1,3-Oxazetidinium Ions? Experiments, Speculations, and Calculations. *Helvetica Chimica Acta*, **2014**, 97, 1177-1203	2	9
98	Electron Density in Quantum Theory. *Structure and Bonding*, **2011**, 99-142	0.9	9
97	Donor- und Acceptor-Stapelwechselwirkungen in einer trans-2-verbrückten C60-Cobalt(II)-tetraphenylporphyrin-Diade. *Angewandte Chemie*, **2006**, 118, 3446-3450	3.6	9
96	Atomistic Approaches in Modern Biology. *Topics in Current Chemistry*, **2007**,		9
95	Transcorrelated density matrix renormalization group. *Journal of Chemical Physics*, **2020**, 153, 164115	3.9	9
94	Explicitly correlated Gaussian functions with shifted-center and projection techniques in pre-Born-Oppenheimer calculations. *Journal of Chemical Physics*, **2018**, 149, 184105	3.9	9
93	Quantum Chemical Spin Densities for Radical Cations of Photosynthetic Pigment Models. *Photochemistry and Photobiology*, **2017**, 93, 815-833	3.6	8
92	Relativistic kinetic-balance condition for explicitly correlated basis functions. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2015**, 48, 245004	1.3	8
91	Nuclear-electronic all-particle density matrix renormalization group. *Journal of Chemical Physics*, **2020**, 152, 204103	3.9	8
90	Structure and dynamics of the radical cation of ethane arising from the Jahn-Teller and pseudo-Jahn-Teller effects. *Physical Chemistry Chemical Physics*, **2018**, 20, 1072-1081	3.6	8
89	Integrated Reaction Path Processing from Sampled Structure Sequences. *Journal of Chemical Theory and Computation*, **2018**, 14, 2052-2062	6.4	8
88	Response to Comment on Accurate frozen-density embedding potentials as a first step towards a subsystem description of covalent bonds [J. Chem. Phys. 135, 027101 (2011)]. *Journal of Chemical Physics*, **2011**, 135, 027102	3.9	8
87	Syntheses, Crystal Structure and Reactivity of Tin(II) Bis[N-(diphenylphosphanyl)(2-pyridylmethyl)amide]. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2009**, 635, 462-470	1.3	8
86	The systems-theoretical view of chemical concepts. *Foundations of Chemistry*, **2003**, 5, 147-163	0.7	8
85	Comment on "gradient-based direct normal-mode analysis" [J. Chem. Phys. 122, 184106 (2005)]. *Journal of Chemical Physics*, **2005**, 123, 117101	3.9	8
84	Self-consistent treatment of the frequency-independent Breit interaction in Dirac-Fock calculations of atomic structures. II. He- and Be-like ions. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2001**, 34, 3133-3156	1.3	8
83	Automated Construction of Quantum-Classical Hybrid Models. *Journal of Chemical Theory and Computation*, **2021**, 17, 3797-3813	6.4	8
82	Mechanistic Consequences of Chelate Ligand Stabilization on Nitrogen Fixation by Yandulov–Schrock-Type Complexes. *ACS Sustainable Chemistry and Engineering*, **2017**, 5, 10527-10537	8.3	7

81	H as a five-body problem described with explicitly correlated Gaussian basis sets. *Journal of Chemical Physics*, **2019**, 151, 154110	3.9	7
80	Coordination and binding geometry of methyl-coenzyme M in the red1m state of methyl-coenzyme M reductase. *Journal of Biological Inorganic Chemistry*, **2008**, 13, 1275-89	3.7	7
79	The gas-phase route from Cp*2P6 to neutral hexaphosphorus. *Chemistry - A European Journal*, **2002**, 8, 5501-6	4.8	7
78	Analysis of spin states, spin barriers, and trans-effects involved in the coordination and stabilization of dinitrogen by biomimetic iron complexes. *Theoretical Chemistry Accounts*, **2005**, 114, 76-83	1.9	7
77	On the Bonding Properties of Diphosphanylmethanide Complexes with the Group-14 Elements Silicon, Germanium, Tin, and Lead in Their Divalent Oxidation States. *European Journal of Inorganic Chemistry*, **1999**, 1999, 1155-1159	2.3	7
76	Complete characterization of the 3p Rydberg complex of a molecular ion: MgAr. I. Observation of the Mg(3p)Ar B state and determination of its structure and dynamics. *Journal of Chemical Physics*, **2020**, 153, 074310	3.9	7
75	Mechanistic insight into organic and industrial transformations: general discussion. *Faraday Discussions*, **2019**, 220, 282-316	3.6	7
74	The Density Matrix Renormalization Group for Strong Correlation in Ground and Excited States **2020**, 205-245		7
73	Systematic dependence of transition-metal coordination energies on density-functional parametrizations. *International Journal of Quantum Chemistry*, **2015**, 115, 90-98	2.1	6
72	Silyl group migration in a P-silylated phosphonium ylide derived from dppm □A combined experimental and theoretical study. *Inorganic Chemistry Communication*, **2013**, 32, 28-31	3.1	6
71	Spin-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, 3671-85	6.4	6
70	Analysis of the asymptotic and short-range behavior of quasilocal Hartree-Fock and Dirac-Fock-Coulomb electron-electron interaction potentials. *Physical Review A*, **2002**, 65,	2.6	6
69	Binding of Reactive Oxygen Species at Fe-S Cubane Clusters. *Chemistry - A European Journal*, **2015**, 21, 19081-9	4.8	5
68	Expansive Quantum Mechanical Exploration of Chemical Reaction Paths.. *Accounts of Chemical Research*, **2021**,	24.3	5
67	Immersive Interactive Quantum Mechanics for Teaching and Learning Chemistry. *Chimia*, **2021**, 75, 45-49	1.3	5
66	Hydrogen-Bonded Networks: Molecular Recognition of Cyclic Alcohols in Enantiopure Alleno-Acetylenic Cage Receptors. *Angewandte Chemie - International Edition*, **2018**, 57, 16296-16301	16.4	5
65	Toward an Inverse Approach for the Design of Small-Molecule Fixating Catalysts. *Materials Research Society Symposia Proceedings*, **2013**, 1524, 101		4
64	Analytical local electron-electron interaction model potentials for atoms. *Physical Review A*, **2002**, 66,	2.6	4

63	Tailored coupled cluster theory in varying correlation regimes. *Journal of Chemical Physics*, **2020**, 153, 244113	3.9	4
62	Semiclassical Dispersion Corrections Efficiently Improve Multiconfigurational Theory with Short-Range Density-Functional Dynamic Correlation. *Journal of Physical Chemistry A*, **2020**, 124, 2834-2841	2.8	3
61	Solvation Free Energies in Subsystem Density Functional Theory.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	3
60	On the Predictive Power of Chemical Concepts. *Chimia*, **2021**, 75, 311-318	1.3	3
59	Tensor network states with three-site correlators. *New Journal of Physics*, **2016**, 18, 113001	2.9	3
58	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	1.3	3
57	Molecule-Specific Uncertainty Quantification in Quantum Chemical Studies. *Israel Journal of Chemistry*, **2022**, 62,	3.4	3
56	Electric transition dipole moment in pre-Born-Oppenheimer molecular structure theory. *Journal of Chemical Physics*, **2014**, 141, 154105	3.9	2
55	Relativistic Quantum Theory of Many-Electron Systems. *Letters in Mathematical Physics*, **2014**, 3-29	0.2	2
54	Chemical Bonding in Open-Shell Transition-Metal Complexes **2014**, 219-252		2
53	Density Functional Theory for Transition Metal Chemistry: The Case of a Water-Splitting Ruthenium Cluster **2011**, 137-163		2
52	Important for the definition of terminology in computational chemistry. *Angewandte Chemie - International Edition*, **2008**, 47, 7171	16.4	2
51	Welche Bedeutung haben Theoretische Konzepte in der Chemie?. *Chemie in Unserer Zeit*, **1999**, 33, 177-185	0.2	2
50	Autonomous Reaction Network Exploration in Homogeneous and Heterogeneous Catalysis.. *Topics in Catalysis*, **2022**, 65, 6-39	2.3	2
49	Excited-State DMRG Made Simple with FEAST.. *Journal of Chemical Theory and Computation*, **2021**,	6.4	2
48	Quantum Proton Effects from Density Matrix Renormalization Group Calculations.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	2
47	Exact decoupling of the relativistic Fock operator **2012**, 205-224		2
46	Sequential Decoupling of Negative-Energy States in Douglas–Kroll–Hess Theory **2015**, 1-16		2

45	New methods: general discussion. *Faraday Discussions*, **2016**, 195, 521-556	3.6	2
44	Computational and theoretical approaches for mechanistic understanding: general discussion. *Faraday Discussions*, **2019**, 220, 464-488	3.6	2
43	Charge-Transfer-Induced Predissociation in Rydberg States of Molecular Cations: MgAr. *Journal of Physical Chemistry A*, **2021**, 125, 6681-6696	2.8	2
42	Special issue on quantum information in chemistry. *International Journal of Quantum Chemistry*, **2015**, 115, 1273-1273	2.1	1
41	Raman Optical Activity Study of the Signatures Associated to (TG)N and (GG)N Conformations of Isotactic Polypropylene Chains using Mode Localization Method **2010**,		1
40	DouglasKrollHess Theory **2009**, 447-478		1
39	Relativistic Effects in Chemistry **2009**, 555-579		1
38	Milde Stickstofffixierung:Was sagt die Theorie?. *Nachrichten Aus Der Chemie*, **2009**, 57, 1093-1096	0.1	1
37	A C2v-Symmetric Barbaralane. *Angewandte Chemie*, **2002**, 114, 3579-3583	3.6	1
36	The apparently unreactive substrate facilitates the electron transfer for dioxygen activation in Rieske dioxygenases.. *Chemistry - A European Journal*, **2022**,	4.8	1
35	Analytically projected, rotationally symmetric, explicitly correlated Gaussian functions with one-axis-shifted centers. *Physical Review A*, **2020**, 102,	2.6	1
34	Experimental Evidence for the Existence of Neutral P(6): A New Allotrope of Phosphorus. *Angewandte Chemie - International Edition*, **1999**, 38, 3513-3515	16.4	1
33	Relativistic Electronic Structure Theory for Molecular Spectroscopy		1
32	The Transferability Limits of Static Benchmarks. *Physical Chemistry Chemical Physics*,	3.6	1
31	Sequential Decoupling of Negative-Energy States in DouglasKrollHess Theory **2017**, 395-410		
30	Theoretical Methods for Supramolecular Chemistry **2012**, 743-793		
29	A: Vector and Tensor Calculus **2009**, 580-587		
28	B: Kinetic Energy in Generalized Coordinates **2009**, 589-590		

27 C: Technical Proofs for Special Relativity **2009**, 591-595

26 D: Relations for Pauli and Dirac Matrices **2009**, 597-600

25 E: Fourier Transformations **2009**, 601-604

24 F: Discretization and Quadrature Schemes **2009**, 605-610

23 G: List of Abbreviations and Acronyms **2009**, 611-612

22 H: List of Symbols **2009**, 613-614

21 General Molecules and Molecular Aggregates **2009**, 385-412

20 Decoupling the Negative-Energy States **2009**, 413-446

19 Elimination Techniques **2009**, 479-501

18 Special Computational Techniques **2009**, 503-515

17 External Electromagnetic Fields and Molecular Properties **2009**, 517-554

16 Elements of Classical Mechanics and Electrodynamics **2009**, 9-50

15 Concepts of Special Relativity **2009**, 51-112

14 Basics of Quantum Mechanics **2009**, 113-150

13 Relativistic Theory of the Electron **2009**, 151-182

12 The Dirac Hydrogen Atom **2009**, 183-224

11 Quantum Electrodynamics **2009**, 227-238

10 First-Quantized Dirac-Based Many-Electron Theory **2009**, 239-313

9	Many-Electron Atoms **2009**, 315-383	
8	Theoretical Methods for Supramolecular Chemistry419-471	
7	Theoretische Chemie 2002. *Nachrichten Aus Der Chemie*, **2003**, 51, 323-329	0.1
6	Structure, Energetics, and Spectroscopy of Models for Enzyme Cofactors **2003**, 163-175	
5	Quantum chemical methods for the vibrational spectroscopy of large molecules **2006**, 1437-1440	
4	On the calculation of properties in the Douglas-Kroll-Hess framework **2006**, 947-952	
3	Physical methods for mechanistic understanding: general discussion. *Faraday Discussions*, **2019**, 220, 144-178	3.6
2	Wasserstoffbrücken-Netzwerke: molekulare Erkennung zyklischer Alkohole in enantiomerenreinen alleno-acetylenischen Käfigrezeptoren. *Angewandte Chemie*, **2018**, 130, 16534-16539	3.6
1	Editorial. *Chimia*, **2014**, 68, 589	1.3