# Markus Reiher

## List of Publications by Year in Descending Order



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| 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 | Autonomous Reaction Network Exploration in Homogeneous and Heterogeneous Catalysis.. *Topics in Catalysis*, **2022**, 65, 6-39 | 2.3 | 2 |
| 367 | The apparently unreactive substrate facilitates the electron transfer for dioxygen activation in Rieske dioxygenases.. *Chemistry - A European Journal*, **2022**, | 4.8 | 1 |
| 366 | Solvation Free Energies in Subsystem Density Functional Theory.. *Journal of Chemical Theory and Computation*, **2022**, | 6.4 | 3 |
| 365 | Quantum Proton Effects from Density Matrix Renormalization Group Calculations.. *Journal of Chemical Theory and Computation*, **2022**, | 6.4 | 2 |
| 364 | Molecule-Specific Uncertainty Quantification in Quantum Chemical Studies. *Israel Journal of Chemistry*, **2022**, 62, | 3.4 | 3 |
| 363 | Expansive Quantum Mechanical Exploration of Chemical Reaction Paths.. *Accounts of Chemical Research*, **2021**, | 24.3 | 5 |
| 362 | Excited-State DMRG Made Simple with FEAST.. *Journal of Chemical Theory and Computation*, **2021**, | 6.4 | 2 |
| 361 | On the Predictive Power of Chemical Concepts. *Chimia*, **2021**, 75, 311-318 | 1.3 | 3 |
| 360 | Automated Construction of Quantum-Classical Hybrid Models. *Journal of Chemical Theory and Computation*, **2021**, 17, 3797-3813 | 6.4 | 8 |
| 359 | Immersive Interactive Quantum Mechanics for Teaching and Learning Chemistry. *Chimia*, **2021**, 75, 45-49 | 1.3 | 5 |
| 358 | Charge-Transfer-Induced Predissociation in Rydberg States of Molecular Cations: MgAr. *Journal of Physical Chemistry A*, **2021**, 125, 6681-6696 | 2.8 | 2 |
| 357 | Quantum computing enhanced computational catalysis. *Physical Review Research*, **2021**, 3, | 3.9 | 17 |
| 356 | Nuclear-electronic all-particle density matrix renormalization group. *Journal of Chemical Physics*, **2020**, 152, 204103 | 3.9 | 8 |
| 355 | Hardware efficient quantum algorithms for vibrational structure calculations. *Chemical Science*, **2020**, 11, 6842-6855 | 9.4 | 19 |
| 354 | Modern quantum chemistry with [Open]Molcas. *Journal of Chemical Physics*, **2020**, 152, 214117 | 3.9 | 106 |
| 353 | 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 |
| 352 | 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 |

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| 351 | The Exploration of Chemical Reaction Networks. *Annual Review of Physical Chemistry*, **2020**, 71, 121-142 | 15.7 | 46 |
| 350 | Self-Parametrizing System-Focused Atomistic Models. *Journal of Chemical Theory and Computation*, **2020**, 16, 1646-1665 | 6.4 | 18 |
| 349 | 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 |
| 348 | Systematic microsolvation approach with a cluster-continuum scheme and conformational sampling. *Journal of Computational Chemistry*, **2020**, 41, 1144-1155 | 3.5 | 28 |
| 347 | Tailored coupled cluster theory in varying correlation regimes. *Journal of Chemical Physics*, **2020**, 153, 244113 | 3.9 | 4 |
| 346 | Transcorrelated density matrix renormalization group. *Journal of Chemical Physics*, **2020**, 153, 164115 | 3.9 | 9 |
| 345 | Analytically projected, rotationally symmetric, explicitly correlated Gaussian functions with one-axis-shifted centers. *Physical Review A*, **2020**, 102, | 2.6 | 1 |
| 344 | 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 |
| 343 | The Density Matrix Renormalization Group for Strong Correlation in Ground and Excited States **2020**, 205-245 | | 7 |
| 342 | OpenMolcas: From Source Code to Insight. *Journal of Chemical Theory and Computation*, **2019**, 15, 5925-5964 | 5.4 | 310 |
| 341 | autoCAS: A Program for Fully Automated Multiconfigurational Calculations. *Journal of Computational Chemistry*, **2019**, 40, 2216-2226 | 3.5 | 40 |
| 340 | Large-Scale Quantum Dynamics with Matrix Product States. *Journal of Chemical Theory and Computation*, **2019**, 15, 3481-3498 | 6.4 | 39 |
| 339 | 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 |
| 338 | Optimization of highly excited matrix product states with an application to vibrational spectroscopy. *Journal of Chemical Physics*, **2019**, 150, 094113 | 3.9 | 20 |
| 337 | 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 |
| 336 | H as a five-body problem described with explicitly correlated Gaussian basis sets. *Journal of Chemical Physics*, **2019**, 151, 154110 | 3.9 | 7 |
| 335 | 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 |
| 334 | Gaussian Process-Based Refinement of Dispersion Corrections. *Journal of Chemical Theory and Computation*, **2019**, 15, 6046-6060 | 6.4 | 25 |

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| 333 | Physical methods for mechanistic understanding: general discussion. *Faraday Discussions*, **2019**, 220, 144-178 | 3.6 | |
| 332 | Mechanistic insight into organic and industrial transformations: general discussion. *Faraday Discussions*, **2019**, 220, 282-316 | 3.6 | 7 |
| 331 | Computational and theoretical approaches for mechanistic understanding: general discussion. *Faraday Discussions*, **2019**, 220, 464-488 | 3.6 | 2 |
| 330 | Exploration of Reaction Pathways and Chemical Transformation Networks. *Journal of Physical Chemistry A*, **2019**, 123, 385-399 | 2.8 | 85 |
| 329 | Mechanism Deduction from Noisy Chemical Reaction Networks. *Journal of Chemical Theory and Computation*, **2019**, 15, 357-370 | 6.4 | 12 |
| 328 | Statistical Analysis of Semiclassical Dispersion Corrections. *Journal of Chemical Theory and Computation*, **2018**, 14, 2480-2494 | 6.4 | 18 |
| 327 | Minimum Energy Paths and Transition States by Curve Optimization. *Journal of Chemical Theory and Computation*, **2018**, 14, 3091-3099 | 6.4 | 11 |
| 326 | The Matter Simulation (R)evolution. *ACS Central Science*, **2018**, 4, 144-152 | 16.8 | 66 |
| 325 | 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 |
| 324 | Calculation of Ligand Dissociation Energies in Large Transition-Metal Complexes. *Journal of Chemical Theory and Computation*, **2018**, 14, 2456-2468 | 6.4 | 48 |
| 323 | Engineering Molecular Iodine Catalysis for Alkyl–Nitrogen Bond Formation. *ACS Catalysis*, **2018**, 8, 3918-3925 | 13.1 | 68 |
| 322 | Integrated Reaction Path Processing from Sampled Structure Sequences. *Journal of Chemical Theory and Computation*, **2018**, 14, 2052-2062 | 6.4 | 8 |
| 321 | 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 |
| 320 | Capture and characterization of a reactive haem carbenoid complex in an artificial metalloenzyme. *Nature Catalysis*, **2018**, 1, 578-584 | 36.5 | 71 |
| 319 | Generalized elimination of the global translation from explicitly correlated Gaussian functions. *Journal of Chemical Physics*, **2018**, 148, 084112 | 3.9 | 10 |
| 318 | Generalized Pauli constraints in small atoms. *Physical Review A*, **2018**, 97, | 2.6 | 13 |
| 317 | 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 |
| 316 | Quantum system partitioning at the single-particle level. *Journal of Chemical Physics*, **2018**, 149, 184104 | 3.9 | 16 |

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| 315 | Wasserstoffbrücken-Netzwerke: molekulare Erkennung zyklischer Alkohole in enantiomerenreinen alleno-acetylenischen Käfigrezeptoren. *Angewandte Chemie*, **2018**, 130, 16534-16539 | 3.6 | |
| 314 | 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 |
| 313 | Semiempirical molecular orbital models based on the neglect of diatomic differential overlap approximation. *International Journal of Quantum Chemistry*, **2018**, 118, e25799 | 2.1 | 29 |
| 312 | Comprehensive Analysis of the Neglect of Diatomic Differential Overlap Approximation. *Journal of Chemical Theory and Computation*, **2018**, 14, 5169-5179 | 6.4 | 12 |
| 311 | Error-Controlled Exploration of Chemical Reaction Networks with Gaussian Processes. *Journal of Chemical Theory and Computation*, **2018**, 14, 5238-5248 | 6.4 | 51 |
| 310 | 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 |
| 309 | Measuring multi-configurational character by orbital entanglement. *Molecular Physics*, **2017**, 115, 2110-2119 | 1.7 | 31 |
| 308 | 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 |
| 307 | Stabilization of activated fragments by shell-wise construction of an embedding environment. *Journal of Computational Chemistry*, **2017**, 38, 1023-1038 | 3.5 | 9 |
| 306 | Second-Order Self-Consistent-Field Density-Matrix Renormalization Group. *Journal of Chemical Theory and Computation*, **2017**, 13, 2533-2549 | 6.4 | 46 |
| 305 | Kooperative Licht-aktivierte Iod- und Photoredox-Katalyse zur Aminierung von C -H-Bindungen. *Angewandte Chemie*, **2017**, 129, 8117-8121 | 3.6 | 53 |
| 304 | 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 |
| 303 | Quantum Chemical Spin Densities for Radical Cations of Photosynthetic Pigment Models. *Photochemistry and Photobiology*, **2017**, 93, 815-833 | 3.6 | 8 |
| 302 | Reliable Estimation of Prediction Uncertainty for Physicochemical Property Models. *Journal of Chemical Theory and Computation*, **2017**, 13, 3297-3317 | 6.4 | 36 |
| 301 | Multiconfigurational Effects in Theoretical Resonance Raman Spectra. *ChemPhysChem*, **2017**, 18, 384-393 | 3.2 | 11 |
| 300 | Context-Driven Exploration of Complex Chemical Reaction Networks. *Journal of Chemical Theory and Computation*, **2017**, 13, 6108-6119 | 6.4 | 49 |
| 299 | 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 |
| 298 | Error Assessment of Computational Models in Chemistry. *Chimia*, **2017**, 71, 202-208 | 1.3 | 23 |

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| 297 | Rigorous Conformational Analysis of Pyrrolidine Enamines with Relevance to Organocatalysis. *Helvetica Chimica Acta*, **2017**, 100, e1700182 | 2 | 17 |
| 296 | 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 |
| 295 | 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 |
| 294 | Vibrational Density Matrix Renormalization Group. *Journal of Chemical Theory and Computation*, **2017**, 13, 3764-3777 | 6.4 | 31 |
| 293 | 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 |
| 292 | Sequential Decoupling of Negative-Energy States in Douglas□Kroll□Hess Theory **2017**, 395-410 | | |
| 291 | Self-adaptive tensor network states with multi-site correlators. *Journal of Chemical Physics*, **2017**, 147, 214111 | 3.9 | 11 |
| 290 | Automated Identification of Relevant Frontier Orbitals for Chemical Compounds and Processes. *Chimia*, **2017**, 71, 170-176 | 1.3 | 53 |
| 289 | Polarizable Embedding Density Matrix Renormalization Group. *Journal of Chemical Theory and Computation*, **2016**, 12, 4242-53 | 6.4 | 20 |
| 288 | The Delicate Balance of Static and Dynamic Electron Correlation. *Journal of Chemical Theory and Computation*, **2016**, 12, 3764-73 | 6.4 | 59 |
| 287 | A Nonorthogonal State-Interaction Approach for Matrix Product State Wave Functions. *Journal of Chemical Theory and Computation*, **2016**, 12, 5881-5894 | 6.4 | 26 |
| 286 | Automated Selection of Active Orbital Spaces. *Journal of Chemical Theory and Computation*, **2016**, 12, 1760-71 | 6.4 | 176 |
| 285 | Tensor network states with three-site correlators. *New Journal of Physics*, **2016**, 18, 113001 | 2.9 | 3 |
| 284 | Nitrous Oxide as a Hydrogen Acceptor for the Dehydrogenative Coupling of Alcohols. *Angewandte Chemie*, **2016**, 128, 1886-1890 | 3.6 | 17 |
| 283 | Real-time feedback from iterative electronic structure calculations. *Journal of Computational Chemistry*, **2016**, 37, 805-12 | 3.5 | 16 |
| 282 | Nitrous Oxide as a Hydrogen Acceptor for the Dehydrogenative Coupling of Alcohols. *Angewandte Chemie - International Edition*, **2016**, 55, 1854-8 | 16.4 | 55 |
| 281 | Calculated Resonance Vibrational Raman Optical Activity Spectra of Naproxen and Ibuprofen. *Journal of Physical Chemistry A*, **2016**, 120, 9740-9748 | 2.8 | 14 |
| 280 | New methods: general discussion. *Faraday Discussions*, **2016**, 195, 521-556 | 3.6 | 2 |

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| 279 | Spin-adapted matrix product states and operators. *Journal of Chemical Physics*, **2016**, 144, 134101 | 3.9 | 51 |
| 278 | Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, **2016**, 37, 506-41 | 3.5 | 1047 |
| 277 | Systematic Error Estimation for Chemical Reaction Energies. *Journal of Chemical Theory and Computation*, **2016**, 12, 2762-73 | 6.4 | 61 |
| 276 | New Approaches for ab initio Calculations of Molecules with Strong Electron Correlation. *Chimia*, **2016**, 70, 244-51 | 1.3 | 74 |
| 275 | Accelerating Wave Function Convergence in Interactive Quantum Chemical Reactivity Studies. *Journal of Chemical Theory and Computation*, **2016**, 12, 1228-35 | 6.4 | 14 |
| 274 | Molecular Propensity as a Driver for Explorative Reactivity Studies. *Journal of Chemical Information and Modeling*, **2016**, 56, 1470-8 | 6.1 | 17 |
| 273 | Uncertainty quantification for quantum chemical models of complex reaction networks. *Faraday Discussions*, **2016**, 195, 497-520 | 3.6 | 47 |
| 272 | 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 |
| 271 | 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 |
| 270 | A stable phosphanyl phosphaketene and its reactivity. *Dalton Transactions*, **2015**, 44, 6431-8 | 4.3 | 60 |
| 269 | Kinetic consequences of introducing a proximal selenocysteine ligand into cytochrome P450cam. *Biochemistry*, **2015**, 54, 6692-703 | 3.2 | 13 |
| 268 | Heuristics-Guided Exploration of Reaction Mechanisms. *Journal of Chemical Theory and Computation*, **2015**, 11, 5712-22 | 6.4 | 102 |
| 267 | Self-consistent embedding of density-matrix renormalization group wavefunctions in a density functional environment. *Journal of Chemical Physics*, **2015**, 142, 044111 | 3.9 | 29 |
| 266 | Density matrix renormalization group with efficient dynamical electron correlation through range separation. *Journal of Chemical Physics*, **2015**, 142, 224108 | 3.9 | 74 |
| 265 | Selection of active spaces for multiconfigurational wavefunctions. *Journal of Chemical Physics*, **2015** , 142, 244104 | 3.9 | 73 |
| 264 | Relativistic kinetic-balance condition for explicitly correlated basis functions. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2015**, 48, 245004 | 1.3 | 8 |
| 263 | Systematic dependence of transition-metal coordination energies on density-functional parametrizations. *International Journal of Quantum Chemistry*, **2015**, 115, 90-98 | 2.1 | 6 |
| 262 | An efficient matrix product operator representation of the quantum chemical Hamiltonian. *Journal of Chemical Physics*, **2015**, 143, 244118 | 3.9 | 100 |

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| 261 | Binding of Reactive Oxygen Species at Fe-S Cubane Clusters. *Chemistry - A European Journal*, **2015**, 21, 19081-9 | 4.8 | 5 |
| 260 | Mode-tracking based stationary-point optimization. *Journal of Computational Chemistry*, **2015**, 36, 1429-38 | 3.5 | 11 |
| 259 | Special issue on quantum information in chemistry. *International Journal of Quantum Chemistry*, **2015**, 115, 1273-1273 | 2.1 | 1 |
| 258 | Sequential Decoupling of Negative-Energy States in Douglas□Kroll□Hess Theory **2015**, 1-16 | | 2 |
| 257 | Inverse quantum chemistry: Concepts and strategies for rational compound design. *International Journal of Quantum Chemistry*, **2014**, 114, 823-837 | 2.1 | 42 |
| 256 | 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 |
| 255 | Electric transition dipole moment in pre-Born-Oppenheimer molecular structure theory. *Journal of Chemical Physics*, **2014**, 141, 154105 | 3.9 | 2 |
| 254 | Studying chemical reactivity in a virtual environment. *Faraday Discussions*, **2014**, 169, 89-118 | 3.6 | 26 |
| 253 | Inaccessibility of the □hydride species in [FeFe] hydrogenases. *Chemical Science*, **2014**, 5, 215-221 | 9.4 | 43 |
| 252 | 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 |
| 251 | Hydrogen-activation mechanism of [Fe] hydrogenase revealed by multi-scale modeling. *Chemical Science*, **2014**, 5, 4474-4482 | 9.4 | 37 |
| 250 | Interactive chemical reactivity exploration. *ChemPhysChem*, **2014**, 15, 3301-19 | 3.2 | 35 |
| 249 | Relativistic Quantum Theory of Many-Electron Systems. *Letters in Mathematical Physics*, **2014**, 3-29 | 0.2 | 2 |
| 248 | 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 |
| 247 | Quantum entanglement in carbon-carbon, carbon-phosphorus and silicon-silicon bonds. *Physical Chemistry Chemical Physics*, **2014**, 16, 8872-80 | 3.6 | 35 |
| 246 | 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 |
| 245 | Chemical Bonding in Open-Shell Transition-Metal Complexes **2014**, 219-252 | | 2 |
| 244 | **2014**, | | 32 |

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| 243 | Determining factors for the accuracy of DMRG in chemistry. *Chimia*, **2014**, 68, 200-3 | 1.3 | 30 |
| 242 | Communication: four-component density matrix renormalization group. *Journal of Chemical Physics*, **2014**, 140, 041101 | 3.9 | 60 |
| 241 | Activation barriers of oxygen transformation at the active site of [FeFe] hydrogenases. *Inorganic Chemistry*, **2014**, 53, 11890-902 | 5.1 | 20 |
| 240 | 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 |
| 239 | Editorial. *Chimia*, **2014**, 68, 589 | 1.3 | |
| 238 | Electric-field effects on the [FeFe]-hydrogenase active site. *Chemical Communications*, **2013**, 49, 8099-101 | 5.8 | 19 |
| 237 | 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 |
| 236 | Local spin analysis and chemical bonding. *Chemistry - A European Journal*, **2013**, 19, 15267-75 | 4.8 | 27 |
| 235 | 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 |
| 234 | Characteristic Raman optical activity signatures of protein ß-sheets. *Journal of Physical Chemistry B*, **2013**, 117, 11943-53 | 3.4 | 23 |
| 233 | Predictors for gases of high electrical strength. *IEEE Transactions on Dielectrics and Electrical Insulation*, **2013**, 20, 856-863 | 2.3 | 38 |
| 232 | Analysis of differences in oxygen sensitivity of Fe-S clusters. *Dalton Transactions*, **2013**, 42, 8729-35 | 4.3 | 22 |
| 231 | Real-time quantum chemistry. *International Journal of Quantum Chemistry*, **2013**, 113, 8-20 | 2.1 | 27 |
| 230 | Formation of a Ph2PCH(BH3)P(BH3)Ph2 ligand via formal 1,2-borane migration. *Chemical Communications*, **2013**, 49, 1121-3 | 5.8 | 12 |
| 229 | 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 |
| 228 | Optimized unrestricted Kohn-Sham potentials from ab initio spin densities. *Journal of Chemical Physics*, **2013**, 138, 044111 | 3.9 | 19 |
| 227 | Elimination of the translational kinetic energy contamination in pre-Born–Oppenheimer calculations. *Molecular Physics*, **2013**, 111, 2086-2092 | 1.7 | 13 |
| 226 | 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 |

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| 225 | Orbital Entanglement in Bond-Formation Processes. *Journal of Chemical Theory and Computation*, **2013**, 9, 2959-73 | 6.4 | 83 |
| 224 | An efficient implementation of two-component relativistic exact-decoupling methods for large molecules. *Journal of Chemical Physics*, **2013**, 138, 184105 | 3.9 | 121 |
| 223 | Theoretical 57Fe Mössbauer spectroscopy for structure elucidation of [Fe] hydrogenase active site intermediates. *Inorganic Chemistry*, **2013**, 52, 14205-15 | 5.1 | 21 |
| 222 | Kinetic modeling of hydrogen conversion at [Fe] hydrogenase active-site models. *Journal of Physical Chemistry B*, **2013**, 117, 4806-17 | 3.4 | 22 |
| 221 | Toward an Inverse Approach for the Design of Small-Molecule Fixating Catalysts. *Materials Research Society Symposia Proceedings*, **2013**, 1524, 101 | | 4 |
| 220 | Structure-Property Relationships of Fe S Clusters. *ChemPlusChem*, **2013**, 78, 1082-1098 | 2.8 | 15 |
| 219 | Exact decoupling of the relativistic Fock operator. *Theoretical Chemistry Accounts*, **2012**, 131, 1 | 1.9 | 183 |
| 218 | 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 |
| 217 | 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 |
| 216 | Spin in density-functional theory. *International Journal of Quantum Chemistry*, **2012**, 112, 3661-3684 | 2.1 | 154 |
| 215 | Entanglement Measures for Single- and Multireference Correlation Effects. *Journal of Physical Chemistry Letters*, **2012**, 3, 3129-35 | 6.4 | 118 |
| 214 | Theoretical Methods for Supramolecular Chemistry **2012**, 743-793 | | |
| 213 | Local relativistic exact decoupling. *Journal of Chemical Physics*, **2012**, 136, 244108 | 3.9 | 68 |
| 212 | Hydrogen Spillover to Nonreducible Supports. *Journal of Physical Chemistry C*, **2012**, 116, 14274-14283 | 3.8 | 45 |
| 211 | Relativistic Douglas–Kroll–Hess theory. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 139-149 | 7.9 | 102 |
| 210 | 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 |
| 209 | Accurate ab Initio Spin Densities. *Journal of Chemical Theory and Computation*, **2012**, 8, 1970-1982 | 6.4 | 70 |
| 208 | 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 |

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| 207 | Hydrogenases and oxygen. *Chemical Science*, **2012**, 3, 1739 | 9.4 | 78 |
| 206 | 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 |
| 205 | Exact decoupling of the relativistic Fock operator **2012**, 205-224 | | 2 |
| 204 | Density Functional Theory for Transition Metal Chemistry: The Case of a Water-Splitting Ruthenium Cluster **2011**, 137-163 | | 2 |
| 203 | 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 |
| 202 | Quantum-information analysis of electronic states of different molecular structures. *Physical Review A*, **2011**, 83, | 2.6 | 125 |
| 201 | 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 |
| 200 | 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 |
| 199 | Construction of CASCI-type wave functions for very large active spaces. *Journal of Chemical Physics*, **2011**, 134, 224101 | 3.9 | 42 |
| 198 | Electron Density in Quantum Theory. *Structure and Bonding*, **2011**, 99-142 | 0.9 | 9 |
| 197 | Mössbauer spectroscopy for heavy elements: a relativistic benchmark study of mercury. *Theoretical Chemistry Accounts*, **2011**, 129, 631-650 | 1.9 | 57 |
| 196 | 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 |
| 195 | Identifying protein turns with vibrational Raman optical activity. *ChemPhysChem*, **2011**, 12, 1165-75 | 3.2 | 13 |
| 194 | Generation of potential energy surfaces in high dimensions and their haptic exploration. *ChemPhysChem*, **2011**, 12, 3204-13 | 3.2 | 21 |
| 193 | New electron correlation theories for transition metal chemistry. *Physical Chemistry Chemical Physics*, **2011**, 13, 6750-9 | 3.6 | 112 |
| 192 | Targeting intermediates of [FeFe]-hydrogenase by CO and CN vibrational signatures. *Inorganic Chemistry*, **2011**, 50, 3888-900 | 5.1 | 48 |
| 191 | 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 |
| 190 | Regioselectivity of H cluster oxidation. *Journal of the American Chemical Society*, **2011**, 133, 20588-603 | 16.4 | 42 |

| | | | |
|---|---|---|---|
| 189 | Catalytic synthesis of vinylphosphanes via calcium-mediated intermolecular hydrophosphanylation of alkynes and butadiynes. *Journal of Organometallic Chemistry*, **2011**, 696, 216-227 | 2.3 | 33 |
| 188 | On the emergence of molecular structure. *Physical Review A*, **2011**, 83, | 2.6 | 44 |
| 187 | Extracting elements of molecular structure from the all-particle wave function. *Journal of Chemical Physics*, **2011**, 135, 204302 | 3.9 | 36 |
| 186 | Enhancement and de-enhancement effects in vibrational resonance Raman optical activity. *Journal of Chemical Physics*, **2010**, 132, 044113 | 3.9 | 50 |
| 185 | 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 |
| 184 | DMRG control using an automated Richardson-type error protocol. *Molecular Physics*, **2010**, 108, 501-512 | 1.7 | 22 |
| 183 | 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 |
| 182 | The Density Matrix Renormalization Group Algorithm in Quantum Chemistry. *Zeitschrift Fur Physikalische Chemie*, **2010**, 224, 583-599 | 3.1 | 136 |
| 181 | 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 |
| 180 | Theoretical Raman optical activity study of the beta domain of rat metallothionein. *Journal of Physical Chemistry B*, **2010**, 114, 1057-63 | 3.4 | 67 |
| 179 | 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 |
| 178 | Basis set representation of the electron density at an atomic nucleus. *Journal of Chemical Physics*, **2010**, 133, 144111 | 3.9 | 27 |
| 177 | Spin Interactions in Cluster Chemistry. *Advances in Inorganic Chemistry*, **2010**, 177-230 | 2.1 | 11 |
| 176 | A unifying structural and electronic concept for Hmd and [FeFe] hydrogenase active sites. *Inorganic Chemistry*, **2010**, 49, 5818-23 | 5.1 | 37 |
| 175 | Complete-graph tensor network states: a new fermionic wave function ansatz for molecules. *New Journal of Physics*, **2010**, 12, 103008 | 2.9 | 70 |
| 174 | Relativistic effects on the Fukui function. *Theoretical Chemistry Accounts*, **2010**, 127, 195-202 | 1.9 | 16 |
| 173 | Prediction of Raman optical activity spectra of chiral 3-acetylcamphorato-cobalt complexes. *ChemPhysChem*, **2010**, 11, 1876-87 | 3.2 | 25 |
| 172 | MOLCAS 7: the next generation. *Journal of Computational Chemistry*, **2010**, 31, 224-47 | 3.5 | 1425 |

| | | | |
|---|---|---|---|
| 171 | Subvalent Organometallic Compounds of the Alkaline Earth Metals in Low Oxidation States. *European Journal of Inorganic Chemistry*, **2010**, 2010, 197-216 | 2.3 | 45 |
| 170 | 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 |
| 169 | Ion dynamics in confined spaces: sodium ion mobility in icosahedral container molecules. *Angewandte Chemie - International Edition*, **2010**, 49, 7465-9 | 16.4 | 13 |
| 168 | A Theoretical Challenge: Transition-Metal Compounds. *Chimia*, **2009**, 63, 140-145 | 1.3 | 54 |
| 167 | Intensity tracking for theoretical infrared spectroscopy of large molecules. *Journal of Chemical Physics*, **2009**, 130, 064105 | 3.9 | 35 |
| 166 | A: Vector and Tensor Calculus **2009**, 580-587 | | |
| 165 | B: Kinetic Energy in Generalized Coordinates **2009**, 589-590 | | |
| 164 | C: Technical Proofs for Special Relativity **2009**, 591-595 | | |
| 163 | D: Relations for Pauli and Dirac Matrices **2009**, 597-600 | | |
| 162 | E: Fourier Transformations **2009**, 601-604 | | |
| 161 | F: Discretization and Quadrature Schemes **2009**, 605-610 | | |
| 160 | G: List of Abbreviations and Acronyms **2009**, 611-612 | | |
| 159 | H: List of Symbols **2009**, 613-614 | | |
| 158 | General Molecules and Molecular Aggregates **2009**, 385-412 | | |
| 157 | Decoupling the Negative-Energy States **2009**, 413-446 | | |
| 156 | Douglas-Kroll-Hess Theory **2009**, 447-478 | | 1 |
| 155 | Elimination Techniques **2009**, 479-501 | | |
| 154 | Special Computational Techniques **2009**, 503-515 | | |

| | | | |
|---|---|---|---|
| 153 | External Electromagnetic Fields and Molecular Properties **2009**, 517-554 | | |
| 152 | Relativistic Effects in Chemistry **2009**, 555-579 | | 1 |
| 151 | Elements of Classical Mechanics and Electrodynamics **2009**, 9-50 | | |
| 150 | Concepts of Special Relativity **2009**, 51-112 | | |
| 149 | Basics of Quantum Mechanics **2009**, 113-150 | | |
| 148 | Relativistic Theory of the Electron **2009**, 151-182 | | |
| 147 | The Dirac Hydrogen Atom **2009**, 183-224 | | |
| 146 | Quantum Electrodynamics **2009**, 227-238 | | |
| 145 | First-Quantized Dirac-Based Many-Electron Theory **2009**, 239-313 | | |
| 144 | Many-Electron Atoms **2009**, 315-383 | | |
| 143 | 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 |
| 142 | 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 |
| 141 | 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 |
| 140 | Intensity-carrying modes in Raman and Raman optical activity spectroscopy. *ChemPhysChem*, **2009**, 10, 2049-57 | 3.2 | 37 |
| 139 | Haptic quantum chemistry. *Journal of Computational Chemistry*, **2009**, 30, 2010-20 | 3.5 | 23 |
| 138 | Electromagnetic fields in relativistic one-particle equations. *Chemical Physics*, **2009**, 356, 205-218 | 2.3 | 22 |
| 137 | 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 |
| 136 | Restrained optimization of broken-symmetry determinants. *International Journal of Quantum Chemistry*, **2009**, 109, 2430-2446 | 2.1 | 23 |

| | | | |
|---|---|---|---|
| 135 | Ligands for dinitrogen fixation at Schrock-type catalysts. *Inorganic Chemistry*, **2009**, 48, 1638-48 | 5.1 | 54 |
| 134 | Theoretical study of dioxygen induced inhibition of [FeFe]-hydrogenase. *Inorganic Chemistry*, **2009**, 48, 7127-40 | 5.1 | 49 |
| 133 | Localizing normal modes in large molecules. *Journal of Chemical Physics*, **2009**, 130, 084106 | 3.9 | 117 |
| 132 | Calculated Raman optical activity spectra of 1,6-anhydro-beta-D-glucopyranose. *Journal of Physical Chemistry A*, **2009**, 113, 8268-77 | 2.8 | 44 |
| 131 | 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 |
| 130 | Milde Stickstofffixierung:Was sagt die Theorie?. *Nachrichten Aus Der Chemie*, **2009**, 57, 1093-1096 | 0.1 | 1 |
| 129 | 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 |
| 128 | Intensity Tracking for Vibrational Spectra of Large Molecules. *Chimia*, **2009**, 63, 270-274 | 1.3 | 13 |
| 127 | **2009**, | | 217 |
| 126 | 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 |
| 125 | Nuclear quadrupole moment of 119Sn. *Journal of Physical Chemistry A*, **2008**, 112, 1666-72 | 2.8 | 36 |
| 124 | The Shell Structure of Atoms. *Journal of Chemical Theory and Computation*, **2008**, 4, 286-96 | 6.4 | 38 |
| 123 | First-principles investigation of the Schrock mechanism of dinitrogen reduction employing the full HIPTN3N ligand. *Inorganic Chemistry*, **2008**, 47, 3634-50 | 5.1 | 104 |
| 122 | Topological analysis of electron densities from Kohn-Sham and subsystem density functional theory. *Journal of Chemical Physics*, **2008**, 128, 044114 | 3.9 | 48 |
| 121 | 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 |
| 120 | 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 |
| 119 | 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 |
| 118 | Selective calculation of high-intensity vibrations in molecular resonance Raman spectra. *Journal of Chemical Physics*, **2008**, 129, 204103 | 3.9 | 34 |

| | | | |
|---|---|---|---|
| 117 | Density matrix renormalization group calculations on relative energies of transition metal complexes and clusters. *Journal of Chemical Physics*, **2008**, 128, 014104 | 3.9 | 147 |
| 116 | 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 |
| 115 | Calculated Raman optical activity signatures of tryptophan side chains. *ChemPhysChem*, **2008**, 9, 2177-80 | 3.2 | 48 |
| 114 | QM/MM vibrational mode tracking. *Journal of Computational Chemistry*, **2008**, 29, 2460-70 | 3.5 | 20 |
| 113 | Important for the definition of terminology in computational chemistry. *Angewandte Chemie - International Edition*, **2008**, 47, 7171 | 16.4 | 2 |
| 112 | (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 |
| 111 | SpinSpin interactions in polynuclear transition-metal complexes. *Chemical Physics Letters*, **2008**, 451, 301-308 | 2.5 | 34 |
| 110 | Analysis of electron density distributions from subsystem density functional theory applied to coordination bonds. *Chemical Physics Letters*, **2008**, 461, 353-359 | 2.5 | 62 |
| 109 | The DouglasKrollHess electron density at an atomic nucleus. *Chemical Physics Letters*, **2008**, 465, 157-164 | 2.5 | 42 |
| 108 | Importance of backbone angles versus amino acid configurations in peptide vibrational Raman optical activity spectra. *Chemical Physics*, **2008**, 343, 200-209 | 2.3 | 31 |
| 107 | Raman optical activity spectra of chiral transition metal complexes. *Chemical Physics*, **2008**, 346, 212-223 | 2.3 | 59 |
| 106 | Finding a needle in a haystack: direct determination of vibrational signatures in complex systems. *New Journal of Chemistry*, **2007**, 31, 818 | 3.6 | 57 |
| 105 | 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 |
| 104 | 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 |
| 103 | Relativistic Effects on the Topology of the Electron Density. *Journal of Chemical Theory and Computation*, **2007**, 3, 2182-97 | 6.4 | 57 |
| 102 | Heavy Grignard reagents: challenges and possibilities of aryl alkaline earth metal compounds. *Chemistry - A European Journal*, **2007**, 13, 6292-306 | 4.8 | 137 |
| 101 | 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 |
| 100 | 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 |

| | | | |
|---|---|---|---|
| 99 | 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 |
| 98 | 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 |
| 97 | 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 |
| 96 | Analytic high-order Douglas-Kroll-Hess electric field gradients. *Journal of Chemical Physics*, **2007**, 127, 074105 | 3.9 | 60 |
| 95 | Decomposition of density matrix renormalization group states into a Slater determinant basis. *Journal of Chemical Physics*, **2007**, 126, 244109 | 3.9 | 73 |
| 94 | 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 |
| 93 | Atomistic Approaches in Modern Biology. *Topics in Current Chemistry*, **2007**, | | 9 |
| 92 | Douglas□Kroll□Hess Theory: a relativistic electrons-only theory for chemistry. *Theoretical Chemistry Accounts*, **2006**, 116, 241-252 | 1.9 | 176 |
| 91 | Intrinsic dinitrogen activation at bare metal atoms. *Angewandte Chemie - International Edition*, **2006**, 45, 6264-88 | 16.4 | 105 |
| 90 | 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 |
| 89 | 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 |
| 88 | 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 |
| 87 | Can Raman optical activity separate axial from local chirality? A theoretical study of helical deca-alanine. *ChemPhysChem*, **2006**, 7, 2189-96 | 3.2 | 69 |
| 86 | 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 |
| 85 | Intrinsische Stickstoff-Aktivierung an □backten□ Metallatomen. *Angewandte Chemie*, **2006**, 118, 6412-6437 | 3.6 | 32 |
| 84 | □Donor- und □Acceptor-Stapelwechselwirkungen in einer trans-2-verbr□kten C60-Cobalt(II)-tetraphenylporphyrin-Diade. *Angewandte Chemie*, **2006**, 118, 3446-3450 | 3.6 | 9 |
| 83 | Chirality-Induced Switch in Hydrogen-Bond Topology: Tetrameric Methyl Lactate Clusters in the Gas Phase. *Angewandte Chemie*, **2006**, 118, 3518-3523 | 3.6 | 22 |
| 82 | Construction of environment states in quantum-chemical density-matrix renormalization group calculations. *Journal of Chemical Physics*, **2006**, 124, 034103 | 3.9 | 47 |

| | | | |
|---|---|---|---|
| 81 | Exact decoupling of the Dirac Hamiltonian. III. Molecular properties. *Journal of Chemical Physics*, **2006**, 124, 64102 | 3.9 | 74 |
| 80 | 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 |
| 79 | First-Principles Approach to Vibrational Spectroscopy of Biomolecules **2006**, 85-132 | | 52 |
| 78 | 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 |
| 77 | Direct targeting of adsorbate vibrations with mode-tracking. *Surface Science*, **2006**, 600, 1891-1900 | 1.8 | 17 |
| 76 | Quantum chemical methods for the vibrational spectroscopy of large molecules **2006**, 1437-1440 | | |
| 75 | On the calculation of properties in the Douglas-Kroll-Hess framework **2006**, 947-952 | | |
| 74 | Relativistic DMRG calculations on the curve crossing of cesium hydride. *Journal of Chemical Physics*, **2005**, 123, 184105 | 3.9 | 58 |
| 73 | Calculation of electric-field gradients based on higher-order generalized Douglas-Kroll transformations. *Journal of Chemical Physics*, **2005**, 122, 204107 | 3.9 | 80 |
| 72 | 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 |
| 71 | Theoretical study of catalytic dinitrogen reduction under mild conditions. *Inorganic Chemistry*, **2005** , 44, 9640-2 | 5.1 | 87 |
| 70 | Understanding the template preorganization step of an artificial arginine receptor. *Journal of the American Chemical Society*, **2005**, 127, 8748-56 | 16.4 | 13 |
| 69 | Basis set and density functional dependence of vibrational Raman optical activity calculations. *Journal of Physical Chemistry A*, **2005**, 109, 7567-74 | 2.8 | 95 |
| 68 | 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 |
| 67 | 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 |
| 66 | 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 |
| 65 | 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 |
| 64 | 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 |

| | | | |
|---|---|---|---|
| 63 | Comment on "gradient-based direct normal-mode analysis" [J. Chem. Phys. 122, 184106 (2005)]. *Journal of Chemical Physics*, **2005**, 123, 117101 | 3.9 | 8 |
| 62 | Convergence behavior of the density-matrix renormalization group algorithm for optimized orbital orderings. *Journal of Chemical Physics*, **2005**, 122, 024107 | 3.9 | 104 |
| 61 | 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 |
| 60 | Comparative analysis of local spin definitions. *Journal of Chemical Physics*, **2005**, 122, 34102 | 3.9 | 77 |
| 59 | TRANSGRESSING THEORY BOUNDARIES: THE GENERALIZED DOUGLAS□KROLL TRANSFORMATION. *Recent Advances in Computational*, **2004**, 137-190 | | 22 |
| 58 | 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 |
| 57 | Combined spectroscopic and theoretical evidence for a persistent end-on copper superoxo complex. *Angewandte Chemie - International Edition*, **2004**, 43, 4360-3 | 16.4 | 150 |
| 56 | Spektroskopischer und theoretischer Nachweis eines best□digen End-on-Kupfersuperoxokomplexes. *Angewandte Chemie*, **2004**, 116, 4460-4464 | 3.6 | 59 |
| 55 | Vibrational center-ligand couplings in transition metal complexes. *Journal of Computational Chemistry*, **2004**, 25, 587-97 | 3.5 | 23 |
| 54 | 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 |
| 53 | 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 |
| 52 | 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 |
| 51 | Properties of WAu12. *Physical Chemistry Chemical Physics*, **2004**, 6, 11-22 | 3.6 | 93 |
| 50 | Convergence characteristics and efficiency of mode-tracking calculations on pre-selected molecular vibrations. *Physical Chemistry Chemical Physics*, **2004**, 6, 4621 | 3.6 | 38 |
| 49 | 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 |
| 48 | 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 |
| 47 | 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 |
| 46 | Mode Tracking of Preselected Vibrations of One-Dimensional Molecular Wires. *Journal of Physical Chemistry A*, **2004**, 108, 2053-2061 | 2.8 | 29 |

| | | | |
|---|---|---|---|
| 45 | Exact decoupling of the Dirac Hamiltonian. I. General theory. *Journal of Chemical Physics*, **2004**, 121, 2037-47 | 3.9 | 406 |
| 44 | QUANTUM CHEMICAL INVESTIGATIONS INTO THE PROBLEM OF BIOLOGICAL NITROGEN FIXATION: SELLMANN-TYPE METAL□SULFUR MODEL COMPLEXES. *Advances in Inorganic Chemistry*, **2004**, 55-100 | 2.1 | 14 |
| 43 | Quantum Chemical Calculation of Raman Intensities for Large Molecules: The Photoisomerization of [{Fe□S4□(PR3)}2(N2H2)] (□S4□□= 1,2-bis(2-Mercaptophenylthio)-Ethane(2-)). *Zeitschrift Fur Physikalische Chemie*, **2003**, 217, 91-104 | 3.1 | 55 |
| 42 | Theoretische Chemie 2002. *Nachrichten Aus Der Chemie*, **2003**, 51, 323-329 | 0.1 | |
| 41 | The systems-theoretical view of chemical concepts. *Foundations of Chemistry*, **2003**, 5, 147-163 | 0.7 | 8 |
| 40 | A Systems Theory for Chemistry. *Foundations of Chemistry*, **2003**, 5, 23-41 | 0.7 | 14 |
| 39 | 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 |
| 38 | 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 |
| 37 | 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 |
| 36 | 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 |
| 35 | 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 |
| 34 | Tetracycline and derivatives□assignment of IR and Raman spectra via DFT calculations. *Physical Chemistry Chemical Physics*, **2003**, 5, 1149-1157 | 3.6 | 70 |
| 33 | Structure, Energetics, and Spectroscopy of Models for Enzyme Cofactors **2003**, 163-175 | | |
| 32 | A C2v-Symmetric Barbaralane. *Angewandte Chemie*, **2002**, 114, 3579-3583 | 3.6 | 1 |
| 31 | 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 |
| 30 | The gas-phase route from Cp*2P6 to neutral hexaphosphorus. *Chemistry - A European Journal*, **2002**, 8, 5501-6 | 4.8 | 7 |
| 29 | A C2v-symmetric barbaralane. *Angewandte Chemie - International Edition*, **2002**, 41, 3429-33 | 16.4 | 11 |
| 28 | 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 |

| | | | |
|---|---|---|---|
| 27 | 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 |
| 26 | 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 |
| 25 | Analytical local electron-electron interaction model potentials for atoms. *Physical Review A*, **2002**, 66, | 2.6 | 4 |
| 24 | Coupled-cluster Raman intensities: Assessment and comparison with multiconfiguration and density functional methods. *Journal of Chemical Physics*, **2002**, 117, 8623-8633 | 3.9 | 37 |
| 23 | Two-component methods and the generalised Douglas–Kroll transformation. *Theoretical and Computational Chemistry*, **2002**, 11, 622-663 | | 25 |
| 22 | 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 |
| 21 | 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 |
| 20 | 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 |
| 19 | The generalized Douglas–Kroll transformation. *Journal of Chemical Physics*, **2002**, 117, 9215-9226 | 3.9 | 558 |
| 18 | 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 |
| 17 | Reparameterization of hybrid functionals based on energy differences of states of different multiplicity. *Theoretical Chemistry Accounts*, **2001**, 107, 48-55 | 1.9 | 1115 |
| 16 | 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 |
| 15 | Dinuclear diazene iron and ruthenium complexes as models for studying nitrogenase activity. *Chemistry - A European Journal*, **2001**, 7, 5195-202 | 4.8 | 50 |
| 14 | 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 |
| 13 | 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 |
| 12 | 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 |
| 11 | A quantum chemical study on the stability of [3n]-allenophanes (n=2–4). *Physical Chemistry Chemical Physics*, **2000**, 2, 2205-2210 | 3.6 | 11 |
| 10 | 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 |

| | | | |
|---|---|---|---|
| 9 | Welche Bedeutung haben Theoretische Konzepte in der Chemie?. *Chemie in Unserer Zeit*, **1999**, 33, 177-185 | 8.1 | 2 |
| 8 | 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 |
| 7 | Experimental Evidence for the Existence of Neutral P6: A New Allotrope of Phosphorus. *Angewandte Chemie - International Edition*, **1999**, 38, 3513-3515 | 16.4 | 15 |
| 6 | 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 |
| 5 | 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 |
| 4 | Isoelectronic Arduengo-Type Carbene Analogues with the Group IIIa Elements Boron, Aluminum, Gallium, and Indium **1998**, 1998, 305-310 | | 62 |
| 3 | Theoretical Methods for Supramolecular Chemistry419-471 | | |
| 2 | Relativistic Electronic Structure Theory for Molecular Spectroscopy | | 1 |
| 1 | The Transferability Limits of Static Benchmarks. *Physical Chemistry Chemical Physics*, | 3.6 | 1 |