Frank Neese

List of Publications by Year in Descending Order

604 papers	59,381 citations	116 h-index	224 g-index
644 ext. papers	67,847 ext. citations	7.3 avg, IF	8.88 L-index

#	Paper	IF	Citations
604	Theoretical analysis of the long-distance limit of NMR chemical shieldings.. *Journal of Chemical Physics*, **2022**, 156, 154115	3.9	0
603	Addressing the System-Size Dependence of the Local Approximation Error in Coupled-Cluster Calculations. *Journal of Physical Chemistry A*, **2021**, 125, 9932-9939	2.8	2
602	An efficient implementation of the NEVPT2 and CASPT2 methods avoiding higher-order density matrices.. *Journal of Chemical Physics*, **2021**, 155, 234104	3.9	2
601	Carbon Monoxide Binding to the Iron-Molybdenum Cofactor of Nitrogenase: a Detailed Quantum Mechanics/Molecular Mechanics Investigation. *Inorganic Chemistry*, **2021**, 60, 18031-18047	5.1	2
600	Cobalt-Catalyzed Hydrosilylation of Carbon Dioxide to the Formic Acid, Formaldehyde, and Methanol Level-How to Control the Catalytic Network?. *Jacs Au*, **2021**, 1, 2058-2069		5
599	Experimental and Theoretical Evidence for an Unusual Almost Triply Degenerate Electronic Ground State of Ferrous Tetraphenylporphyrin. *Inorganic Chemistry*, **2021**, 60, 4966-4985	5.1	5
598	Comparison of Many-Particle Representations for Selected Configuration Interaction: II. Numerical Benchmark Calculations. *Journal of Chemical Theory and Computation*, **2021**, 17, 2868-2885	6.4	6
597	Productive Alkyne Metathesis with "Canopy Catalysts" Mandates Pseudorotation. *Journal of the American Chemical Society*, **2021**, 143, 5643-5648	16.4	10
596	Structure-Spectroscopy Correlations for Intermediate Q of Soluble Methane Monooxygenase: Insights from QM/MM Calculations. *Journal of the American Chemical Society*, **2021**, 143, 6560-6577	16.4	6
595	DLPNO-MP2 second derivatives for the computation of polarizabilities and NMR shieldings. *Journal of Chemical Physics*, **2021**, 154, 164110	3.9	9
594	Coexistence of Two Different Distorted Octahedral [MnF] Sites in K [MnF]: Manifestation in Spectroscopy and Magnetism. *Chemistry - A European Journal*, **2021**, 27, 9801-9813	4.8	5
593	Computational molecular spectroscopy. *Nature Reviews Methods Primers*, **2021**, 1,		18
592	Converged Structural and Spectroscopic Properties for Refined QM/MM Models of Azurin. *Inorganic Chemistry*, **2021**, 60, 7399-7412	5.1	3
591	Fragment-Based Local Coupled Cluster Embedding Approach for the Quantification and Analysis of Noncovalent Interactions: Exploring the Many-Body Expansion of the Local Coupled Cluster Energy. *Journal of Chemical Theory and Computation*, **2021**, 17, 3348-3359	6.4	4
590	Approximations of density matrices in N-electron valence state second-order perturbation theory (NEVPT2). I. Revisiting the NEVPT2 construction. *Journal of Chemical Physics*, **2021**, 154, 214111	3.9	7
589	Approximations of density matrices in N-electron valence state second-order perturbation theory (NEVPT2). II. The full rank NEVPT2 (FR-NEVPT2) formulation. *Journal of Chemical Physics*, **2021**, 154, 214113	3.9	5
588	Spectroscopic and Theoretical Study on Siloxy-Based Molybdenum and Tungsten Alkylidyne Catalysts for Alkyne Metathesis. *ACS Catalysis*, **2021**, 11, 9086-9101	13.1	3

587	Nudged Elastic Band Method for Molecular Reactions Using Energy-Weighted Springs Combined with Eigenvector Following. *Journal of Chemical Theory and Computation*, **2021**, 17, 4929-4945	6.4	22
586	Unraveling individual host-guest interactions in molecular recognition from first principles quantum mechanics: Insights into the nature of nicotinic acetylcholine receptor agonist binding. *Journal of Computational Chemistry*, **2021**, 42, 293-302	3.5	3
585	Chlorophyll excitation energies and structural stability of the CP47 antenna of photosystem II: a case study in the first-principles simulation of light-harvesting complexes. *Chemical Science*, **2021**, 12, 4463-4476	9.4	3
584	A Quantum Chemistry View on Two Archetypical Paramagnetic Pentacoordinate Nickel(II) Complexes Offers a Fresh Look on Their NMR Spectra. *Inorganic Chemistry*, **2021**, 60, 2068-2075	5.1	9
583	Unveiling the complex pattern of intermolecular interactions responsible for the stability of the DNA duplex. *Chemical Science*, **2021**, 12, 12785-12793	9.4	2
582	Redesigning donor-acceptor Stenhouse adduct photoswitches through a joint experimental and computational study. *Chemical Science*, **2021**, 12, 2916-2924	9.4	5
581	Robust magnetic anisotropy of a monolayer of hexacoordinate Fe(II) complexes assembled on Cu(111). *Inorganic Chemistry Frontiers*, **2021**, 8, 2395-2404	6.8	3
580	How Can We Predict Accurate Electrochromic Shifts for Biochromophores? A Case Study on the Photosynthetic Reaction Center. *Journal of Chemical Theory and Computation*, **2021**, 17, 1858-1873	6.4	7
579	Comparison of many-particle representations for selected-CI I: A tree based approach. *Journal of Computational Chemistry*, **2021**, 42, 982-1005	3.5	14
578	Implicit solvation in domain based pair natural orbital coupled cluster (DLPNO-CCSD) theory. *Journal of Computational Chemistry*, **2021**, 42, 1959-1973	3.5	2
577	An improved chain of spheres for exchange algorithm. *Journal of Chemical Physics*, **2021**, 155, 104109	3.9	5
576	A Joint Venture of Ab Initio Molecular Dynamics, Coupled Cluster Electronic Structure Methods, and Liquid-State Theory to Compute Accurate Isotropic Hyperfine Constants of Nitroxide Probes in Water. *Journal of Chemical Theory and Computation*, **2021**, 17, 6366-6386	6.4	2
575	Cluster-in-Molecule Local Correlation Method with an Accurate Distant Pair Correction for Large Systems. *Journal of Chemical Theory and Computation*, **2021**, 17, 756-766	6.4	7
574	Effect of Spin-Orbit Coupling on Phonon-Mediated Magnetic Relaxation in a Series of Zero-Valent Vanadium, Niobium, and Tantalum Isocyanide Complexes. *Inorganic Chemistry*, **2021**, 60, 18553-18560	5.1	2
573	First-Principles Study of Optical Absorption Energies, Ligand Field and Spin-Hamiltonian Parameters of Cr Ions in Emeralds.. *Inorganic Chemistry*, **2021**,	5.1	1
572	The first microsolvation step for furans: New experiments and benchmarking strategies. *Journal of Chemical Physics*, **2020**, 152, 164303	3.9	14
571	Performance of density functional theory and orbital-optimised second-order perturbation theory methods for geometries and singlet–triplet state splittings of aryl-carbenes. *Molecular Physics*, **2020**, 118, e1764644	1.7	10
570	Spin-chemical effects on intramolecular photoinduced charge transfer reactions in bisphenanthroline copper(i)-viologen dyad assemblies. *Chemical Science*, **2020**, 11, 5511-5525	9.4	

569	The ORCA quantum chemistry program package. *Journal of Chemical Physics*, **2020**, 152, 224108	3.9	479
568	All-electron scalar relativistic basis sets for the elements Rb-Xe. *Journal of Computational Chemistry* , **2020**, 41, 1842-1849	3.5	28
567	An alternative choice of the zeroth-order Hamiltonian in CASPT2 theory. *Journal of Chemical Physics* , **2020**, 152, 214110	3.9	6
566	Mechanism of L-edge x-ray magnetic circular dichroism intensity from quantum chemical calculations and experiment-A case study on V/V complexes. *Journal of Chemical Physics*, **2020**, 152, 114107	3.9	4
565	Strong and Confined Acids Control Five Stereogenic Centers in Catalytic Asymmetric Diels-Alder Reactions of Cyclohexadienones with Cyclopentadiene. *Angewandte Chemie - International Edition*, **2020**, 59, 12347-12351	16.4	16
564	Detailed Pair Natural Orbital-Based Coupled Cluster Studies of Spin Crossover Energetics. *Journal of Chemical Theory and Computation*, **2020**, 16, 2224-2235	6.4	35
563	Sulfur vs. Selenium as Bridging Ligand in Di-Iron Complexes: A Theoretical Analysis. *European Journal of Inorganic Chemistry*, **2020**, 2020, 1525-1538	2.3	4
562	Starke und sterisch begrenzte S□uren kontrollieren f□f stereogene Zentren in der katalytischen asymmetrischen Diels-Alder-Reaktion von Cyclohexadienonen mit Cyclopentadien. *Angewandte Chemie*, **2020**, 132, 12446-12450	3.6	5
561	Linear scaling perturbative triples correction approximations for open-shell domain-based local pair natural orbital coupled cluster singles and doubles theory [DLPNO-CCSD(T/T)]. *Journal of Chemical Physics*, **2020**, 152, 024116	3.9	22
560	Unveiling the Delicate Balance of Steric and Dispersion Interactions in Organocatalysis Using High-Level Computational Methods. *Journal of the American Chemical Society*, **2020**, 142, 3613-3625	16.4	34
559	Improvement of Ab Initio Ligand Field Theory by Means of Multistate Perturbation Theory. *Journal of Physical Chemistry A*, **2020**, 124, 1025-1037	2.8	11
558	The combination of multipartitioning of the Hamiltonian with canonical Van Vleck perturbation theory leads to a Hermitian variant of quasidegenerate N-electron valence perturbation theory. *Journal of Chemical Physics*, **2020**, 152, 014109	3.9	5
557	Walter Thiel (1949□2019). *Angewandte Chemie*, **2020**, 132, 1398-1399	3.6	
556	Walter Thiel (1949-2019). *Angewandte Chemie - International Edition*, **2020**, 59, 1382-1383	16.4	2
555	Where Is the Fluoro Wall?: A Quantum Chemical Investigation. *Inorganic Chemistry*, **2020**, 59, 1556-1565	5.1	4
554	Dispersion Forces Drive the Formation of Uranium-Alkane Adducts. *Journal of the American Chemical Society*, **2020**, 142, 1864-1870	16.4	9
553	Effect of the Solute Cavity on the Solvation Energy and its Derivatives within the Framework of the Gaussian Charge Scheme. *Journal of Computational Chemistry*, **2020**, 41, 922-939	3.5	33
552	Formyltetrahydrofolate Decarbonylase Synthesizes the Active Site CO Ligand of O-Tolerant [NiFe] Hydrogenase. *Journal of the American Chemical Society*, **2020**, 142, 1457-1464	16.4	12

551	Comprehensive Benchmark Results for the Domain Based Local Pair Natural Orbital Coupled Cluster Method (DLPNO-CCSD(T)) for Closed- and Open-Shell Systems. *Journal of Physical Chemistry A*, **2020**, 124, 90-100	2.8	90
550	Unveiling the Photophysical Properties of Boron-dipyrromethene Dyes Using a New Accurate Excited State Coupled Cluster Method. *Journal of Chemical Theory and Computation*, **2020**, 16, 564-575	6.4	30
549	Computation of NMR Shielding Constants for Solids Using an Embedded Cluster Approach with DFT, Double-Hybrid DFT, and MP2. *Journal of Chemical Theory and Computation*, **2020**, 16, 6950-6967	6.4	12
548	Protein Matrix Control of Reaction Center Excitation in Photosystem II. *Journal of the American Chemical Society*, **2020**, 142, 18174-18190	16.4	21
547	MQM 2019 Introduction. *Molecular Physics*, **2020**, 118, e1839187	1.7	
546	Fe Mssbauer parameters from domain based local pair-natural orbital coupled-cluster theory. *Journal of Chemical Physics*, **2020**, 153, 204101	3.9	2
545	Double-hybrid density functional theory for g-tensor calculations using gauge including atomic orbitals. *Journal of Chemical Physics*, **2020**, 153, 054105	3.9	5
544	Strong Electronic and Magnetic Coupling in M (M = Ni, Cu) Clusters via Direct Orbital Interactions between Low-Coordinate Metal Centers. *Journal of the American Chemical Society*, **2020**, 142, 19161-19169	16.4	11
543	A case study of density functional theory and domain-based local pair natural orbital coupled cluster for vibrational effects on EPR hyperfine coupling constants: vibrational perturbation theory versus ab initio molecular dynamics. *Molecular Physics*, **2020**, 118, e1797916	1.7	4
542	Explicitly correlated coupled cluster method for accurate treatment of open-shell molecules with hundreds of atoms. *Journal of Chemical Physics*, **2020**, 153, 094105	3.9	4
541	Accurate Computation of the Absorption Spectrum of Chlorophyll with Pair Natural Orbital Coupled Cluster Methods. *Journal of Physical Chemistry B*, **2020**, 124, 8761-8771	3.4	27
540	Solution of a Puzzle: High-Level Quantum-Chemical Treatment of Pseudocontact Chemical Shifts Confirms Classic Semiempirical Theory. *Journal of Physical Chemistry Letters*, **2020**, 11, 8735-8744	6.4	13
539	Isolation of a Homoleptic Non-oxo Mo(V) Alkoxide Complex: Synthesis, Structure, and Electronic Properties of Penta--Butoxymolybdenum. *Journal of the American Chemical Society*, **2020**, 142, 16392-16402	16.4	8
538	Extrapolation to the Limit of a Complete Pair Natural Orbital Space in Local Coupled-Cluster Calculations. *Journal of Chemical Theory and Computation*, **2020**, 16, 6142-6149	6.4	14
537	Magnetic Properties and Electronic Structure of the = 2 Complex [Mn{(OPPh)N}] Showing Field-Induced Slow Magnetization Relaxation. *Inorganic Chemistry*, **2020**, 59, 13281-13294	5.1	3
536	Ligand Field Theory and Angular Overlap Model Based Analysis of the Electronic Structure of Homovalent Iron-Sulfur Dimers. *Inorganic Chemistry*, **2020**, 59, 984-995	5.1	15
535	HFLD: A Nonempirical London Dispersion-Corrected Hartree-Fock Method for the Quantification and Analysis of Noncovalent Interaction Energies of Large Molecular Systems *Journal of Chemical Theory and Computation*, **2019**, 15, 5894-5907	6.4	17
534	A Series of Iron Nitrosyl Complexes {Fe-NO} and a Fleeting {Fe-NO} Intermediate en Route to a Metalacyclic Iron Nitrosoalkane. *Journal of the American Chemical Society*, **2019**, 141, 17217-17235	16.4	16

533	Reduction of CO by a masked two-coordinate cobalt(i) complex and characterization of a proposed oxodicobalt(ii) intermediate. *Chemical Science*, **2019**, 10, 918-929	9.4	23
532	Microsolvation of the Redox-Active Tyrosine-D in Photosystem II: Correlation of Energetics with EPR Spectroscopy and Oxidation-Induced Proton Transfer. *Journal of the American Chemical Society* , **2019**, 141, 3217-3231	16.4	12
531	Perturbative triples correction to domain-based local pair natural orbital variants of Mukherjee's state specific coupled cluster method. *Physical Chemistry Chemical Physics*, **2019**, 21, 5022-5038	3.6	7
530	Local Energy Decomposition of Open-Shell Molecular Systems in the Domain-Based Local Pair Natural Orbital Coupled Cluster Framework. *Journal of Chemical Theory and Computation*, **2019**, 15, 1616-1632	6.4	46
529	Efficient simulation of overtones and combination bands in resonant Raman spectra. *Journal of Chemical Physics*, **2019**, 150, 214102	3.9	11
528	A domain-based local pair natural orbital implementation of the equation of motion coupled cluster method for electron attached states. *Journal of Chemical Physics*, **2019**, 150, 164123	3.9	35
527	Analytical gradient for the domain-based local pair natural orbital second order Møller-Plesset perturbation theory method (DLPNO-MP2). *Journal of Chemical Physics*, **2019**, 150, 164102	3.9	18
526	Multilayer Approach to the IP-EOM-DLPNO-CCSD Method: Theory, Implementation, and Application. *Journal of Chemical Theory and Computation*, **2019**, 15, 2265-2277	6.4	15
525	New Boron(III) Blue Emitters for All-Solution Processed OLEDs: Molecular Design Assisted by Theoretical Modeling. *European Journal of Inorganic Chemistry*, **2019**, 2019, 2247-2257	2.3	12
524	Spectroscopic and Quantum Chemical Investigation of Benzene-1,2-dithiolate-Coordinated Diiron Complexes with Relevance to Dinitrogen Activation. *Inorganic Chemistry*, **2019**, 58, 5111-5125	5.1	5
523	Spin-dependent properties in the framework of the dynamic correlation dressed complete active space method. *Journal of Chemical Physics*, **2019**, 150, 104104	3.9	17
522	Comparison of multireference ab initio wavefunction methodologies for X-ray absorption edges: A case study on [Fe(II/III)Cl] molecules. *Journal of Chemical Physics*, **2019**, 150, 104106	3.9	16
521	London dispersion effects in the coordination and activation of alkanes in Ecomplexes: a local energy decomposition study. *Physical Chemistry Chemical Physics*, **2019**, 21, 11569-11577	3.6	30
520	Probing Magnetic Excitations in CoII Single-Molecule Magnets by Inelastic Neutron Scattering. *European Journal of Inorganic Chemistry*, **2019**, 2019, 1055-1055	2.3	
519	Physical Nature of Differential Spin-State Stabilization of Carbenes by Hydrogen and Halogen Bonding: A Domain-Based Pair Natural Orbital Coupled Cluster Study. *Journal of Physical Chemistry A*, **2019**, 123, 5081-5090	2.8	11
518	Efficient implementation of the analytical second derivatives of hartree-fock and hybrid DFT energies within the framework of the conductor-like polarizable continuum model. *Journal of Computational Chemistry*, **2019**, 40, 1816-1828	3.5	14
517	Predicting Phosphorescence Rates of Light Organic Molecules Using Time-Dependent Density Functional Theory and the Path Integral Approach to Dynamics. *Journal of Chemical Theory and Computation*, **2019**, 15, 1896-1904	6.4	77
516	A perturbation-based super-CI approach for the orbital optimization of a CASSCF wave function. *Journal of Computational Chemistry*, **2019**, 40, 1463-1470	3.5	15

515	Five-coordinate Mn intermediate in the activation of nature's water splitting cofactor. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 16841-16846	11.5	33
514	Computational Design of Near-Infrared Fluorescent Organic Dyes Using an Accurate New Wave Function Approach. *Journal of Physical Chemistry Letters*, **2019**, 10, 4822-4828	6.4	20
513	Implications of structural heterogeneity for the electronic structure of the final oxygen-evolving intermediate in photosystem II. *Journal of Inorganic Biochemistry*, **2019**, 199, 110797	4.2	13
512	Accurate Band Gap Predictions of Semiconductors in the Framework of the Similarity Transformed Equation of Motion Coupled Cluster Theory. *Inorganic Chemistry*, **2019**, 58, 9303-9315	5.1	29
511	Planar three-coordinate iron sulfide in a synthetic [4Fe-3S] cluster with biomimetic reactivity. *Nature Chemistry*, **2019**, 11, 1019-1025	17.6	25
510	Conversion of a Fleeting Open-Shell Iron Nitride into an Iron Nitrosyl. *Angewandte Chemie*, **2019**, 131, 17753-17757	3.6	2
509	Conversion of a Fleeting Open-Shell Iron Nitride into an Iron Nitrosyl. *Angewandte Chemie - International Edition*, **2019**, 58, 17589-17593	16.4	6
508	Insights into Single-Molecule-Magnet Behavior from the Experimental Electron Density of Linear Two-Coordinate Iron Complexes. *Inorganic Chemistry*, **2019**, 58, 3211-3218	5.1	21
507	Probing Magnetic Excitations in CoII Single-Molecule Magnets by Inelastic Neutron Scattering. *European Journal of Inorganic Chemistry*, **2019**, 2019, 1119-1127	2.3	9
506	Electron Paramagnetic Resonance Signature of Tetragonal Low Spin Iron(V)-Nitrido and -Oxo Complexes Derived from the Electronic Structure Analysis of Heme and Non-Heme Archetypes. *Journal of the American Chemical Society*, **2019**, 141, 2421-2434	16.4	29
505	Chemistry and Quantum Mechanics in 2019: Give Us Insight and Numbers. *Journal of the American Chemical Society*, **2019**, 141, 2814-2824	16.4	60
504	Accurate Ionization Potentials, Electron Affinities and Electronegativities of Single-Walled Carbon Nanotubes by State-of-the-Art Local Coupled-Cluster Theory. *Bulletin of the Chemical Society of Japan*, **2019**, 92, 170-174	5.1	2
503	Effect of Electron Correlation on Intermolecular Interactions: A Pair Natural Orbitals Coupled Cluster Based Local Energy Decomposition Study. *Journal of Chemical Theory and Computation*, **2019**, 15, 215-228	6.4	52
502	Palladium-catalysed electrophilic aromatic C-H fluorination. *Nature*, **2018**, 554, 511-514	50.4	92
501	Formation of Agostic Structures Driven by London Dispersion. *Angewandte Chemie - International Edition*, **2018**, 57, 4760-4764	16.4	43
500	Comparison and combination of "direct" and fragment based local correlation methods: Cluster in molecules and domain based local pair natural orbital perturbation and coupled cluster theories. *Journal of Chemical Physics*, **2018**, 148, 124117	3.9	31
499	Formation of Agostic Structures Driven by London Dispersion. *Angewandte Chemie*, **2018**, 130, 4850-4854	3.6	6
498	The [U2F12]2−Anion of Sr[U2F12]. *Angewandte Chemie*, **2018**, 130, 2964-2968	3.6	5

497	Electronic Structure and Spin Multiplicity of Iron Tetraphenylporphyrins in Their Reduced States as Determined by a Combination of Resonance Raman Spectroscopy and Quantum Chemistry. *Inorganic Chemistry*, **2018**, 57, 2141-2148	5.1	30
496	Domain-Based Local Pair Natural Orbital Version of Mukherjee's State-Specific Coupled Cluster Method. *Journal of Chemical Theory and Computation*, **2018**, 14, 1370-1382	6.4	24
495	Communication: Exact analytical derivatives for the domain-based local pair natural orbital MP2 method (DLPNO-MP2). *Journal of Chemical Physics*, **2018**, 148, 031101	3.9	22
494	On the theoretical prediction of fluorescence rates from first principles using the path integral approach. *Journal of Chemical Physics*, **2018**, 148, 034104	3.9	66
493	Communication: An improved linear scaling perturbative triples correction for the domain based local pair-natural orbital based singles and doubles coupled cluster method [DLPNO-CCSD(T)]. *Journal of Chemical Physics*, **2018**, 148, 011101	3.9	224
492	The [U F] Anion of Sr[U F]. *Angewandte Chemie - International Edition*, **2018**, 57, 2914-2918	16.4	9
491	Accelerating the coupled-cluster singles and doubles method using the chain-of-sphere approximation. *Molecular Physics*, **2018**, 116, 1428-1434	1.7	15
490	Pair Natural Orbital Restricted Open-Shell Configuration Interaction (PNO-ROCIS) Approach for Calculating X-ray Absorption Spectra of Large Chemical Systems. *Journal of Physical Chemistry A*, **2018**, 122, 1215-1227	2.8	20
489	The furan microsolvation blind challenge for quantum chemical methods: First steps. *Journal of Chemical Physics*, **2018**, 148, 014301	3.9	34
488	Self-Consistent Field Calculation of Nuclear Magnetic Resonance Chemical Shielding Constants Using Gauge-Including Atomic Orbitals and Approximate Two-Electron Integrals. *Journal of Chemical Theory and Computation*, **2018**, 14, 619-637	6.4	37
487	NAMD goes quantum: an integrative suite for hybrid simulations. *Nature Methods*, **2018**, 15, 351-354	21.6	88
486	Software update: the ORCA program system, version 4.0. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1327	7.9	2068
485	Restricted Open-Shell Configuration Interaction Singles Study on M- and L-edge X-ray Absorption Spectroscopy of Solid Chemical Systems. *Journal of Chemical Theory and Computation*, **2018**, 14, 4320-4334	6.4	11
484	Challenges in Multireference Perturbation Theory for the Calculations of the g-Tensor of First-Row Transition-Metal Complexes. *Journal of Chemical Theory and Computation*, **2018**, 14, 4662-4677	6.4	38
483	Accurate spin-densities based on the domain-based local pair-natural orbital coupled-cluster theory. *Journal of Chemical Physics*, **2018**, 149, 034104	3.9	39
482	Efficient and Accurate Prediction of Nuclear Magnetic Resonance Shielding Tensors with Double-Hybrid Density Functional Theory. *Journal of Chemical Theory and Computation*, **2018**, 14, 4756-4771	6.4	40
481	Electronic Structure Contributions of Non-Heme Oxo-Iron(V) Complexes to the Reactivity. *Journal of the American Chemical Society*, **2018**, 140, 9531-9544	16.4	53
480	Accurate Spin-State Energetics for Aryl Carbenes. *Journal of Chemical Theory and Computation*, **2018**, 14, 4733-4746	6.4	17

479	Ab Initio Wave Function-Based Determination of Element Specific Shifts for the Efficient Calculation of X-ray Absorption Spectra of Main Group Elements and First Row Transition Metals. *Journal of Chemical Theory and Computation*, **2018**, 14, 3686-3702	6.4	28
478	Toward Accurate QM/MM Reaction Barriers with Large QM Regions Using Domain Based Pair Natural Orbital Coupled Cluster Theory. *Journal of Chemical Theory and Computation*, **2018**, 14, 3524-3531	6.4	28
477	Exploring the Accuracy of a Low Scaling Similarity Transformed Equation of Motion Method for Vertical Excitation Energies. *Journal of Chemical Theory and Computation*, **2018**, 14, 72-91	6.4	61
476	A linear cobalt(II) complex with maximal orbital angular momentum from a non-Aufbau ground state. *Science*, **2018**, 362,	33.3	164
475	Computational Insights into Chemical Reactivity and Road to Catalyst Design: The Paradigm of CO2 Hydrogenation **2018**, 33-48		
474	Computational Studies on Vibronic Coupling in Single Molecule Magnets: Impact on the Mechanism of Magnetic Relaxation. *Journal of Physics: Conference Series*, **2018**, 1148, 012006	0.3	2
473	An efficient pair natural orbital based configuration interaction scheme for the calculation of open-shell ionization potentials. *Journal of Chemical Physics*, **2018**, 149, 114108	3.9	5
472	Scalable and Highly Diastereo- and Enantioselective Catalytic Diels-Alder Reaction of Unsaturated Methyl Esters. *Journal of the American Chemical Society*, **2018**, 140, 12671-12676	16.4	30
471	Chemical Tuning of Magnetic Exchange Couplings Using Broken-Symmetry Density Functional Theory. *Inorganic Chemistry*, **2018**, 57, 12769-12776	5.1	19
470	London Dispersion Interactions in Pnictogen Cations [ECl] and [E=E] (E=P, As, Sb) Supported by Anionic N-Heterocyclic Carbenes. *Chemistry - A European Journal*, **2018**, 24, 18922-18932	4.8	28
469	Enhanced Electrophilicity of Heterobimetallic Bi-Rh Paddlewheel Carbene Complexes: A Combined Experimental, Spectroscopic, and Computational Study. *Journal of the American Chemical Society*, **2018**, 140, 13042-13055	16.4	41
468	Local energy decomposition analysis of hydrogen-bonded dimers within a domain-based pair natural orbital coupled cluster study. *Beilstein Journal of Organic Chemistry*, **2018**, 14, 919-929	2.5	39
467	Investigations of the Magnetic and Spectroscopic Properties of V(III) and V(IV) Complexes. *Inorganic Chemistry*, **2018**, 57, 6421-6438	5.1	8
466	A near-linear scaling equation of motion coupled cluster method for ionized states. *Journal of Chemical Physics*, **2018**, 148, 244101	3.9	32
465	Spin-phonon couplings in transition metal complexes with slow magnetic relaxation. *Nature Communications*, **2018**, 9, 2572	17.4	58
464	Revisiting the Mssbauer Isomer Shifts of the FeMoco Cluster of Nitrogenase and the Cofactor Charge. *Inorganic Chemistry*, **2017**, 56, 1470-1477	5.1	79
463	Automatic active space selection for the similarity transformed equations of motion coupled cluster method. *Journal of Chemical Physics*, **2017**, 146, 074103	3.9	42
462	Magneto-Structural Correlations in Pseudotetrahedral Forms of the [Co(SPh)] Complex Probed by Magnetometry, MCD Spectroscopy, Advanced EPR Techniques, and ab Initio Electronic Structure Calculations. *Inorganic Chemistry*, **2017**, 56, 3102-3118	5.1	58

461	Pair natural orbital and canonical coupled cluster reaction enthalpies involving light to heavy alkali and alkaline earth metals: the importance of sub-valence correlation. *Physical Chemistry Chemical Physics*, **2017**, 19, 9374-9391	3.6	36
460	Tuning Magnetic Anisotropy Through Ligand Substitution in Five-Coordinate Co(II) Complexes. *Inorganic Chemistry*, **2017**, 56, 5253-5265	5.1	23
459	SparseMaps-A systematic infrastructure for reduced scaling electronic structure methods. V. Linear scaling explicitly correlated coupled-cluster method with pair natural orbitals. *Journal of Chemical Physics*, **2017**, 146, 174108	3.9	84
458	A new near-linear scaling, efficient and accurate, open-shell domain-based local pair natural orbital coupled cluster singles and doubles theory. *Journal of Chemical Physics*, **2017**, 146, 164105	3.9	194
457	Multilevel Approaches within the Local Pair Natural Orbital Framework. *Journal of Chemical Theory and Computation*, **2017**, 13, 3198-3207	6.4	20
456	A simple scheme for calculating approximate transition moments within the equation of motion expectation value formalism. *Journal of Chemical Physics*, **2017**, 146, 214111	3.9	9
455	Generation, Spectroscopic, and Chemical Characterization of an Octahedral Iron(V)-Nitrido Species with a Neutral Ligand Platform. *Journal of the American Chemical Society*, **2017**, 139, 9168-9177	16.4	33
454	Electronic Structure and Magnetic Anisotropy of an Unsaturated Cyclopentadienyl Iron(I) Complex with 15 Valence Electrons. *Angewandte Chemie - International Edition*, **2017**, 56, 7995-7999	16.4	22
453	Nonclassical Single-State Reactivity of an Oxo-Iron(IV) Complex Confined to Triplet Pathways. *Journal of the American Chemical Society*, **2017**, 139, 8939-8949	16.4	62
452	EPR/ENDOR and Theoretical Study of the Jahn-Teller-Active [HIPTNN]MoL Complexes (L = N, NH). *Inorganic Chemistry*, **2017**, 56, 6906-6919	5.1	11
451	Arbitrary Angular Momentum Electron Repulsion Integrals with Graphical Processing Units: Application to the Resolution of Identity Hartree-Fock Method. *Journal of Chemical Theory and Computation*, **2017**, 13, 3160-3170	6.4	21
450	A toolchain for the automatic generation of computer codes for correlated wavefunction calculations. *Journal of Computational Chemistry*, **2017**, 38, 1853-1868	3.5	14
449	Covalency and chemical bonding in transition metal complexes: An ab initio based ligand field perspective. *Coordination Chemistry Reviews*, **2017**, 344, 2-25	23.2	108
448	Electronic Structure of a Formal Iron(0) Porphyrin Complex Relevant to CO Reduction. *Inorganic Chemistry*, **2017**, 56, 4746-4751	5.1	56
447	Ligandenumlagerungen an Fe/S-Cofaktoren: langsame Isomerisierung eines biomimetischen [2Fe-2S]-Clusters. *Angewandte Chemie*, **2017**, 129, 4960-4964	3.6	2
446	Quantum Chemistry and EPR Parameters **2017**, 1-22		20
445	Ligand Rearrangements at Fe/S Cofactors: Slow Isomerization of a Biomimetic [2Fe-2S] Cluster. *Angewandte Chemie - International Edition*, **2017**, 56, 4882-4886	16.4	11
444	Structural models of the biological oxygen-evolving complex: achievements, insights, and challenges for biomimicry. *Green Chemistry*, **2017**, 19, 2309-2325	10	55

443	Automatic Generation of Auxiliary Basis Sets. *Journal of Chemical Theory and Computation*, **2017**, 13, 554-562	6.4	205
442	Time-Resolved Electron Paramagnetic Resonance and Theoretical Investigations of Metal-Free Room-Temperature Triplet Emitters. *Journal of the American Chemical Society*, **2017**, 139, 12968-12975	16.4	14
441	Revisiting the Electronic Structure of FeS Monomers Using ab Initio Ligand Field Theory and the Angular Overlap Model. *Inorganic Chemistry*, **2017**, 56, 10418-10436	5.1	10
440	A Restricted Open Configuration Interaction with Singles Method To Calculate Valence-to-Core Resonant X-ray Emission Spectra: A Case Study. *Inorganic Chemistry*, **2017**, 56, 11819-11836	5.1	20
439	The First State in the Catalytic Cycle of the Water-Oxidizing Enzyme: Identification of a Water-Derived Hydroxo Bridge. *Journal of the American Chemical Society*, **2017**, 139, 14412-14424	16.4	49
438	Vollautomatisierte quantenchemische Berechnung von Spin-Spin- gekoppelten magnetischen Kernspinresonanzspektren. *Angewandte Chemie*, **2017**, 129, 14958-14964	3.6	25
437	Fully Automated Quantum-Chemistry-Based Computation of Spin-Spin-Coupled Nuclear Magnetic Resonance Spectra. *Angewandte Chemie - International Edition*, **2017**, 56, 14763-14769	16.4	107
436	Explicitly correlated N-electron valence state perturbation theory (NEVPT2-F12). *Journal of Chemical Physics*, **2017**, 147, 064110	3.9	13
435	High-Level Spectroscopy, Quantum Chemistry, and Catalysis: Not just a Passing Fad. *Angewandte Chemie - International Edition*, **2017**, 56, 11003-11010	16.4	27
434	Kombination von hochwertiger Spektroskopie, Quantenchemie und Katalyse: nicht nur eine Modeerscheinung. *Angewandte Chemie*, **2017**, 129, 11147-11154	3.6	6
433	Surface hopping dynamics including intersystem crossing using the algebraic diagrammatic construction method. *Journal of Chemical Physics*, **2017**, 147, 184109	3.9	23
432	[OsF] : Molecular Models for Spin-Orbit Entangled Phenomena. *Chemistry - A European Journal*, **2017**, 23, 11244-11248	4.8	16
431	A combined experimental and theoretical spectroscopic protocol for determination of the structure of heterogeneous catalysts: developing the information content of the resonance Raman spectra of M1 MoVO. *Chemical Science*, **2017**, 8, 6338-6353	9.4	7
430	Ab Initio Ligand-Field Theory Analysis and Covalency Trends in Actinide and Lanthanide Free Ions and Octahedral Complexes. *Inorganic Chemistry*, **2017**, 56, 8802-8816	5.1	68
429	Treating Subvalence Correlation Effects in Domain Based Pair Natural Orbital Coupled Cluster Calculations: An Out-of-the-Box Approach. *Journal of Chemical Theory and Computation*, **2017**, 13, 3220-3227	5.4	29
428	Elektronische Struktur und magnetische Anisotropie eines ungesättigten Cyclopentadienyleisen(I)-Komplexes mit 15 Valenzelektronen. *Angewandte Chemie*, **2017**, 129, 8107-8112	3.6	5
427	Understanding the Role of Dispersion in Frustrated Lewis Pairs and Classical Lewis Adducts: A Domain-Based Local Pair Natural Orbital Coupled Cluster Study. *Chemistry - A European Journal*, **2017**, 23, 865-873	4.8	66
426	Binding free energies in the SAMPL5 octa-acid host-guest challenge calculated with DFT-D3 and CCSD(T). *Journal of Computer-Aided Molecular Design*, **2017**, 31, 87-106	4.2	18

425	A dynamic correlation dressed complete active space method: Theory, implementation, and preliminary applications. *Journal of Chemical Physics*, **2017**, 147, 234109	3.9	29
424	Similarity transformed equation of motion coupled-cluster theory based on an unrestricted Hartree-Fock reference for applications to high-spin open-shell systems. *Journal of Chemical Physics* , **2017**, 147, 174104	3.9	12
423	Cobalt Phosphino-□minopyridine-Catalyzed Hydrofunctionalization of Alkenes: Catalyst Development and Mechanistic Analysis. *Organometallics*, **2016**, 35, 2900-2914	3.8	28
422	Decomposition of Intermolecular Interaction Energies within the Local Pair Natural Orbital Coupled Cluster Framework. *Journal of Chemical Theory and Computation*, **2016**, 12, 4778-4792	6.4	159
421	Hydrogen evolution in [NiFe] hydrogenases and related biomimetic systems: similarities and differences. *Physical Chemistry Chemical Physics*, **2016**, 18, 24681-92	3.6	12
420	High-Valent Iron-Oxo and -Nitrido Complexes: Bonding and Reactivity. *Israel Journal of Chemistry*, **2016**, 56, 763-772	3.4	24
419	Effect of Conjugation Pathway in Metal-Free Room-Temperature Dual Singlet-Triplet Emitters for Organic Light-Emitting Diodes. *Journal of Physical Chemistry Letters*, **2016**, 7, 4802-4808	6.4	30
418	Homoleptic Two-Coordinate Silylamido Complexes of Chromium(I), Manganese(I), and Cobalt(I). *Chemistry - A European Journal*, **2016**, 22, 1668-74	4.8	45
417	A realistic in silico model for structure/function studies of molybdenum-copper CO dehydrogenase. *Journal of Biological Inorganic Chemistry*, **2016**, 21, 491-9	3.7	14
416	Recent developments in biological water oxidation. *Current Opinion in Chemical Biology*, **2016**, 31, 113-9	9.7	87
415	A four-coordinate cobalt(II) single-ion magnet with coercivity and a very high energy barrier. *Nature Communications*, **2016**, 7, 10467	17.4	295
414	Improved Segmented All-Electron Relativistically Contracted Basis Sets for the Lanthanides. *Journal of Chemical Theory and Computation*, **2016**, 12, 1148-56	6.4	62
413	In search of metal hydrides: an X-ray absorption and emission study of [NiFe] hydrogenase model complexes. *Physical Chemistry Chemical Physics*, **2016**, 18, 10688-99	3.6	27
412	A five-coordinate Mn(iv) intermediate in biological water oxidation: spectroscopic signature and a pivot mechanism for water binding. *Chemical Science*, **2016**, 7, 72-84	9.4	134
411	Electronic Structures of the [Fe(N2)(SiP(iPr)3)](+1/0/-1) Electron Transfer Series: A Counterintuitive Correlation between Isomer Shifts and Oxidation States. *Inorganic Chemistry*, **2016**, 55, 3468-74	5.1	37
410	A unified view on heterogeneous and homogeneous catalysts through a combination of spectroscopy and quantum chemistry. *Faraday Discussions*, **2016**, 188, 181-97	3.6	26
409	Redox potential tuning by redox-inactive cations in nature's water oxidizing catalyst and synthetic analogues. *Physical Chemistry Chemical Physics*, **2016**, 18, 10739-50	3.6	29
408	Spin State as a Marker for the Structural Evolution of Nature's Water-Splitting Catalyst. *Inorganic Chemistry*, **2016**, 55, 488-501	5.1	70

407	Non-Noble Metal Catalysis NoNoMeCat. *Impact*, **2016**, 2016, 20-22	0.3	
406	SparseMaps--A systematic infrastructure for reduced-scaling electronic structure methods. III. Linear-scaling multireference domain-based pair natural orbital N-electron valence perturbation theory. *Journal of Chemical Physics*, **2016**, 144, 094111	3.9	105
405	SparseMaps--A systematic infrastructure for reduced-scaling electronic structure methods. IV. Linear-scaling second-order explicitly correlated energy with pair natural orbitals. *Journal of Chemical Physics*, **2016**, 144, 144109	3.9	77
404	Comparison of fully internally and strongly contracted multireference configuration interaction procedures. *Journal of Chemical Physics*, **2016**, 145, 054104	3.9	39
403	Analytic energy derivatives for the calculation of the first-order molecular properties using the domain-based local pair-natural orbital coupled-cluster theory. *Journal of Chemical Physics*, **2016**, 145, 114101	3.9	47
402	Towards a pair natural orbital coupled cluster method for excited states. *Journal of Chemical Physics*, **2016**, 145, 034102	3.9	90
401	Speeding up equation of motion coupled cluster theory with the chain of spheres approximation. *Journal of Chemical Physics*, **2016**, 144, 034102	3.9	52
400	Sparse maps--A systematic infrastructure for reduced-scaling electronic structure methods. II. Linear scaling domain based pair natural orbital coupled cluster theory. *Journal of Chemical Physics*, **2016**, 144, 024109	3.9	489
399	Spectroscopic Evidence for the Two C-H-Cleaving Intermediates of Aspergillus nidulans Isopenicillin N Synthase. *Journal of the American Chemical Society*, **2016**, 138, 8862-74	16.4	83
398	Unravelling the Molecular Origin of the Regiospecificity in Extradiol Catechol Dioxygenases. *Inorganic Chemistry*, **2016**, 55, 3853-64	5.1	31
397	Periodic Trends in Lanthanide Compounds through the Eyes of Multireference ab Initio Theory. *Inorganic Chemistry*, **2016**, 55, 4457-69	5.1	64
396	Ionization Energies and Aqueous Redox Potentials of Organic Molecules: Comparison of DFT, Correlated ab Initio Theory and Pair Natural Orbital Approaches. *Journal of Chemical Theory and Computation*, **2016**, 12, 2272-84	6.4	68
395	Toward Rational Design of 3d Transition Metal Catalysts for CO2 Hydrogenation Based on Insights into Hydricity-Controlled Rate-Determining Steps. *Inorganic Chemistry*, **2016**, 55, 5438-44	5.1	57
394	Magnetic Circular Dichroism Evidence for an Unusual Electronic Structure of a Tetracarbene-Oxoiron(IV) Complex. *Journal of the American Chemical Society*, **2016**, 138, 14312-14325	16.4	43
393	Coupled Cluster Method with Single and Double Excitations Tailored by Matrix Product State Wave Functions. *Journal of Physical Chemistry Letters*, **2016**, 7, 4072-4078	6.4	59
392	Surface Adsorption Energetics Studied with "Gold Standard" Wave-Function-Based Ab Initio Methods: Small-Molecule Binding to TiO(110). *Journal of Physical Chemistry Letters*, **2016**, 7, 4207-4212	6.4	70
391	A Structurally Characterized Nonheme Cobalt-Hydroperoxo Complex Derived from Its Superoxo Intermediate via Hydrogen Atom Abstraction. *Journal of the American Chemical Society*, **2016**, 138, 14186-14189	16.4	54
390	The ligand field of the azido ligand: insights into bonding parameters and magnetic anisotropy in a Co(II)-azido complex. *Journal of the American Chemical Society*, **2015**, 137, 1993-2005	16.4	108

389	Magnetic circular dichroism and computational study of mononuclear and dinuclear iron(IV) complexes. *Chemical Science*, **2015**, 6, 2909-2921	9.4	22
388	Exploring the Accuracy Limits of Local Pair Natural Orbital Coupled-Cluster Theory. *Journal of Chemical Theory and Computation*, **2015**, 11, 1525-39	6.4	389
387	Control in the Rate-Determining Step Provides a Promising Strategy To Develop New Catalysts for CO2 Hydrogenation: A Local Pair Natural Orbital Coupled Cluster Theory Study. *Inorganic Chemistry* , **2015**, 54, 7192-8	5.1	72
386	Efficient implementation of the analytic second derivatives of Hartree–Fock and hybrid DFT energies: a detailed analysis of different approximations. *Molecular Physics*, **2015**, 113, 1961-1977	1.7	27
385	Characterization of Oxygen Bridged Manganese Model Complexes Using Multifrequency (17)O-Hyperfine EPR Spectroscopies and Density Functional Theory. *Journal of Physical Chemistry B*, **2015**, 119, 13904-21	3.4	19
384	Free reaction enthalpy profile of the Schrock cycle derived from density functional theory calculations on the full [Mo(HIPT)N3N] catalyst. *Inorganic Chemistry*, **2015**, 54, 9248-55	5.1	38
383	Is It Possible To Obtain Coupled Cluster Quality Energies at near Density Functional Theory Cost? Domain-Based Local Pair Natural Orbital Coupled Cluster vs Modern Density Functional Theory. *Journal of Chemical Theory and Computation*, **2015**, 11, 4054-63	6.4	184
382	Distal Histidine Modulates the Unusual O-Binding of Nitrite to Myoglobin: Evidence from the Quantum Chemical Analysis of EPR Parameters. *Inorganic Chemistry*, **2015**, 54, 7209-17	5.1	15
381	A Local Pair Natural Orbital-Based Multireference Mukherjee's Coupled Cluster Method. *Journal of Chemical Theory and Computation*, **2015**, 11, 3104-14	6.4	53
380	Dioxygen Activation and Catalytic Reduction to Hydrogen Peroxide by a Thiolate-Bridged Dimanganese(II) Complex with a Pendant Thiol. *Journal of the American Chemical Society*, **2015**, 137, 8644-53	16.4	44
379	Calcium and heterometallic manganese-calcium complexes supported by tripodal pyridine-carboxylate ligands: structural, EPR and theoretical investigations. *Dalton Transactions*, **2015**, 44, 12757-70	4.3	14
378	Domain Based Pair Natural Orbital Coupled Cluster Studies on Linear and Folded Alkane Chains. *Journal of Chemical Theory and Computation*, **2015**, 11, 2137-43	6.4	45
377	Magnetic Transitions in Iron Porphyrin Halides by Inelastic Neutron Scattering and Ab Initio Studies of Zero-Field Splittings. *Inorganic Chemistry*, **2015**, 54, 9790-801	5.1	42
376	Spin Isomers and Ligand Isomerization in a Three-Coordinate Cobalt(I) Carbonyl Complex. *Journal of the American Chemical Society*, **2015**, 137, 10689-99	16.4	18
375	A trans-1,2 End-On Disulfide-Bridged Iron-Tetracarbene Dimer and Its Electronic Structure. *Inorganic Chemistry*, **2015**, 54, 9770-6	5.1	14
374	Magneto-Structural Correlations in a Series of Pseudotetrahedral [Co(II)(XR)4](2-) Single Molecule Magnets: An ab Initio Ligand Field Study. *Inorganic Chemistry*, **2015**, 54, 9948-61	5.1	88
373	Six-electron reduction of nitrite to ammonia by cytochrome c nitrite reductase: insights from density functional theory studies. *Inorganic Chemistry*, **2015**, 54, 9303-16	5.1	50
372	How Accurately Can Extended X-ray Absorption Spectra Be Predicted from First Principles? Implications for Modeling the Oxygen-Evolving Complex in Photosystem II. *Journal of the American Chemical Society*, **2015**, 137, 12815-34	16.4	22

371	Hydride bridge in [NiFe]-hydrogenase observed by nuclear resonance vibrational spectroscopy. *Nature Communications*, **2015**, 6, 7890	17.4	73
370	Direct Observation of Very Large Zero-Field Splitting in a Tetrahedral Ni(II)Se4 Coordination Complex. *Journal of the American Chemical Society*, **2015**, 137, 12923-8	16.4	33
369	Molybdenum L-Edge XAS Spectra of MoFe Nitrogenase. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2015**, 641, 65-71	1.3	30
368	Finding the Reactive Electron in Paramagnetic Systems: A Critical Evaluation of Accuracies for EPR Spectroscopy and Density Functional Theory Using 1,3,5-Triphenyl Verdazyl Radical as a Testcase. *Applied Magnetic Resonance*, **2015**, 46, 117-139	0.8	6
367	First principles approach to the electronic structure, magnetic anisotropy and spin relaxation in mononuclear 3d-transition metal single molecule magnets. *Coordination Chemistry Reviews*, **2015**, 289-290, 177-214	23.2	217
366	Sparse maps—A systematic infrastructure for reduced-scaling electronic structure methods. I. An efficient and simple linear scaling local MP2 method that uses an intermediate basis of pair natural orbitals. *Journal of Chemical Physics*, **2015**, 143, 034108	3.9	169
365	Resolving the Manganese Oxidation States in the Oxygen-evolving Catalyst of Natural Photosynthesis. *Israel Journal of Chemistry*, **2015**, 55, 1219-1232	3.4	21
364	Artificial photosynthesis: understanding water splitting in nature. *Interface Focus*, **2015**, 5, 20150009	3.9	47
363	Molecular and Electronic Structures of Homoleptic Six-Coordinate Cobalt(I) Complexes of 2,2':6',2?-Terpyridine, 2,2'-Bipyridine, and 1,10-Phenanthroline. An Experimental and Computational Study. *Inorganic Chemistry*, **2015**, 54, 12002-18	5.1	42
362	Mössbauer and computational investigation of a functional [NiFe] hydrogenase model complex. *Chemical Communications*, **2015**, 51, 2099-102	5.8	21
361	The discovery of Mo(III) in FeMoco: reuniting enzyme and model chemistry. *Journal of Biological Inorganic Chemistry*, **2015**, 20, 447-60	3.7	63
360	Hydrogen bond network between amino acid radical intermediates on the proton-coupled electron transfer pathway of E. coli class Ia ribonucleotide reductase. *Journal of the American Chemical Society*, **2015**, 137, 289-98	16.4	56
359	EPR and Quantum Chemical Investigation of a Bioinspired Hydrogenase Model with a Redox-Active Ligand in the First Coordination Sphere. *Organometallics*, **2015**, 34, 995-1000	3.8	12
358	Metal oxidation states in biological water splitting. *Chemical Science*, **2015**, 6, 1676-1695	9.4	225
357	Bio-inspired mechanistic insights into CO_2 reduction. *Current Opinion in Chemical Biology*, **2015**, 25, 103-9	9.7	69
356	New insights into the nature of observable reaction intermediates in cytochrome P450 NO reductase by using a combination of spectroscopy and quantum mechanics/molecular mechanics calculations. *Chemistry - A European Journal*, **2014**, 20, 1602-14	4.8	24
355	Does a higher metal oxidation state necessarily imply higher reactivity toward H-atom transfer? A computational study of C-H bond oxidation by high-valent iron-oxo and -nitrido complexes. *Dalton Transactions*, **2014**, 43, 6079-86	4.3	41
354	Structure, ligands and substrate coordination of the oxygen-evolving complex of photosystem II in the S2 state: a combined EPR and DFT study. *Physical Chemistry Chemical Physics*, **2014**, 16, 11877-92	3.6	66

353	Communication: multireference equation of motion coupled cluster: a transform and diagonalize approach to electronic structure. *Journal of Chemical Physics*, **2014**, 140, 081102	3.9	40
352	The first tyrosyl radical intermediate formed in the S2-S3 transition of photosystem II. *Physical Chemistry Chemical Physics*, **2014**, 16, 11901-10	3.6	60
351	Decay of iron(V) nitride complexes by a N-N bond-coupling reaction in solution: a combined spectroscopic and theoretical analysis. *Angewandte Chemie - International Edition*, **2014**, 53, 8727-31	16.4	25
350	Chemical applications carried out by local pair natural orbital based coupled-cluster methods. *Chemical Society Reviews*, **2014**, 43, 5032-41	58.5	102
349	Oxygen-evolving Photosystem II **2014**, 1-13		4
348	Restricted open-shell configuration interaction cluster calculations of the L-edge X-ray absorption study of TiO(2) and CaF(2) solids. *Inorganic Chemistry*, **2014**, 53, 6374-85	5.1	45
347	Spectroscopic and Quantum Chemical Study of the Ni(PPh2NC6H4CH2P(O)(OEt)22)2 Electrocatalyst for Hydrogen Production with Emphasis on the NiI Oxidation State. *Journal of Physical Chemistry C*, **2014**, 118, 2350-2360	3.8	15
346	Mechanism of Olefin Asymmetric Hydrogenation Catalyzed by Iridium Phosphino-Oxazoline: A Pair Natural Orbital Coupled Cluster Study. *Journal of Chemical Theory and Computation*, **2014**, 10, 1099-108	6.4	52
345	On the reaction mechanism of the complete intermolecular O2 transfer between mononuclear nickel and manganese complexes with macrocyclic ligands. *Chemistry - A European Journal*, **2014**, 20, 13296-304	4.8	4
344	Geminal-spanning orbitals make explicitly correlated reduced-scaling coupled-cluster methods robust, yet simple. *Journal of Chemical Physics*, **2014**, 141, 054106	3.9	33
343	A first-principles approach to the calculation of the on-site zero-field splitting in polynuclear transition metal complexes. *Inorganic Chemistry*, **2014**, 53, 11785-93	5.1	28
342	L-edge X-ray absorption study of mononuclear vanadium complexes and spectral predictions using a restricted open shell configuration interaction ansatz. *Physical Chemistry Chemical Physics*, **2014**, 16, 264-76	3.6	64
341	Identification of a spin-coupled Mo(III) in the nitrogenase iron□molybdenum cofactor. *Chemical Science*, **2014**, 5, 3096-3103	9.4	131
340	Synthesis, detailed characterization, and theoretical understanding of mononuclear chromium(III)-containing polyoxotungstates [Cr(III)(HX(V)W□□□□? (X = P, As) with exceptionally large magnetic anisotropy. *Inorganic Chemistry*, **2014**, 53, 9274-83	5.1	19
339	Excitation wavelength dependent O2 release from copper(II)-superoxide compounds: laser flash-photolysis experiments and theoretical studies. *Journal of the American Chemical Society*, **2014**, 136, 1260-3	16.4	27
338	Low-energy spectrum of iron-sulfur clusters directly from many-particle quantum mechanics. *Nature Chemistry*, **2014**, 6, 927-33	17.6	197
337	Electronic structural flexibility of heterobimetallic Mn/Fe cofactors: R2lox and R2c proteins. *Journal of the American Chemical Society*, **2014**, 136, 13399-409	16.4	31
336	A well-defined terminal vanadium(III) oxo complex. *Inorganic Chemistry*, **2014**, 53, 11388-95	5.1	23

335	Photosynthesis. Electronic structure of the oxygen-evolving complex in photosystem II prior to O-O bond formation. *Science*, **2014**, 345, 804-8	33.3	363
334	Combined Experimental and Ab Initio Multireference Configuration Interaction Study of the Resonant Inelastic X-ray Scattering Spectrum of CO2. *Journal of Physical Chemistry C*, **2014**, 118, 20163-20175	4.8	28
333	The mechanism of homogeneous CO2 reduction by Ni(cyclam): product selectivity, concerted proton-electron transfer and C-O bond cleavage. *Inorganic Chemistry*, **2014**, 53, 7500-7	5.1	124
332	Correlated Ab Initio and Density Functional Studies on H2 Activation by FeO(.). *Journal of Chemical Theory and Computation*, **2014**, 10, 3807-20	6.4	75
331	All-electron basis sets for heavy elements. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 363-374	7.9	26
330	Synthetic and computational evaluation of regiodivergent epoxide opening for diol and polyol synthesis. *Chemistry - an Asian Journal*, **2014**, 9, 2289-94	4.5	16
329	K□mainline X-ray emission spectroscopy as an experimental probe of metal-ligand covalency. *Journal of the American Chemical Society*, **2014**, 136, 9453-63	16.4	92
328	Pulsed electron paramagnetic resonance spectroscopy of (33)S-labeled molybdenum cofactor in catalytically active bioengineered sulfite oxidase. *Inorganic Chemistry*, **2014**, 53, 961-71	5.1	9
327	Abbau von Nitridoeisen(V)-Komplexen durch N-N-Kupplung in L□sung: spektroskopische und theoretische Analyse. *Angewandte Chemie*, **2014**, 126, 8872-8876	3.6	9
326	The static response function in Kohn-Sham theory: an appropriate basis for its matrix representation in case of finite AO basis sets. *Journal of Chemical Physics*, **2014**, 141, 134106	3.9	7
325	The iron-sulfur core in Rieske proteins is not symmetric. *Journal of Biological Inorganic Chemistry*, **2014**, 19, 1287-93	3.7	3
324	SORCI for photochemical and thermal reaction paths: A benchmark study. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 84-98	2	16
323	Heme-bound nitroxyl, hydroxylamine, and ammonia ligands as intermediates in the reaction cycle of cytochrome c nitrite reductase: a theoretical study. *Journal of Biological Inorganic Chemistry*, **2014**, 19, 97-112	3.7	19
322	Assessment of n-Electron Valence State Perturbation Theory for Vertical Excitation Energies. *Journal of Chemical Theory and Computation*, **2013**, 9, 3567-80	6.4	90
321	Theoretical spectroscopy of the Ni(II) intermediate states in the catalytic cycle and the activation of [NiFe] hydrogenases. *ChemBioChem*, **2013**, 14, 1898-905	3.8	48
320	Convergence of QM/MM and Cluster Models for the Spectroscopic Properties of the Oxygen-Evolving Complex in Photosystem II. *Journal of Chemical Theory and Computation*, **2013**, 9, 3832-42	6.4	50
319	X-Ray Spectroscopy **2013**, 427-439		2
318	Ammonia binding to the oxygen-evolving complex of photosystem II identifies the solvent-exchangeable oxygen bridge (□xo) of the manganese tetramer. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 15561-6	11.5	130

317	High-resolution molybdenum K-edge X-ray absorption spectroscopy analyzed with time-dependent density functional theory. *Physical Chemistry Chemical Physics*, **2013**, 15, 20911-20	3.6	58
316	Experimental and computational X-ray emission spectroscopy as a direct probe of protonation states in oxo-bridged Mn(IV) dimers relevant to redox-active metalloproteins. *Inorganic Chemistry*, **2013**, 52, 12915-22	5.1	49
315	The protonation states of oxo-bridged Mn(IV) dimers resolved by experimental and computational Mn K pre-edge X-ray absorption spectroscopy. *Inorganic Chemistry*, **2013**, 52, 12904-14	5.1	41
314	Structural and spectroscopic investigation of an anilinosalen cobalt complex with relevance to hydrogen production. *Inorganic Chemistry*, **2013**, 52, 14428-38	5.1	21
313	Natural triple excitations in local coupled cluster calculations with pair natural orbitals. *Journal of Chemical Physics*, **2013**, 139, 134101	3.9	876
312	Robust fitting techniques in the chain of spheres approximation to the Fock exchange: The role of the complementary space. *Journal of Chemical Physics*, **2013**, 139, 094111	3.9	59
311	Electronic structure analysis of multistate reactivity in transition metal catalyzed reactions: the case of C-H bond activation by non-heme iron(IV)-oxo cores. *Physical Chemistry Chemical Physics*, **2013**, 15, 8017-30	3.6	138
310	Electronic structure of the unique [4Fe-3S] cluster in O2-tolerant hydrogenases characterized by 57Fe Mossbauer and EPR spectroscopy. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 483-8	11.5	50
309	A theoretical study of zero-field splitting in Fe(IV)S6 (S = 1) and Fe(III)S6 (S = 1/2) core complexes, [FeIV(Et2dtc)3□(mnt)n](n□1)□and [FeIII(Et2dtc)3□(mnt)n]n□(n = 0, 1, 2, 3): The origin of the magnetic anisotropy. *Coordination Chemistry Reviews*, **2013**, 257, 27-41	23.2	18
308	Preference towards five-coordination in Ti silicalite-1 upon molecular adsorption. *ChemPhysChem*, **2013**, 14, 79-83	3.2	47
307	An efficient and near linear scaling pair natural orbital based local coupled cluster method. *Journal of Chemical Physics*, **2013**, 138, 034106	3.9	890
306	A combined high-field EPR and quantum chemical study on a weakly ferromagnetically coupled dinuclear Mn(III) complex. A complete analysis of the EPR spectrum beyond the strong coupling limit. *Physical Chemistry Chemical Physics*, **2013**, 15, 223-34	3.6	18
305	Slow magnetization dynamics in a series of two-coordinate iron(II) complexes. *Chemical Science*, **2013**, 4, 125-138	9.4	455
304	A theoretical analysis of chemical bonding, vibronic coupling, and magnetic anisotropy in linear iron(II) complexes with single-molecule magnet behavior. *Chemical Science*, **2013**, 4, 139-156	9.4	213
303	Biological water oxidation. *Accounts of Chemical Research*, **2013**, 46, 1588-96	24.3	407
302	Hydrogen-bonding effects on the reactivity of [X-Fe(III)-O-Fe(IV)?O] (X = OH, F) complexes toward C-H bond cleavage. *Inorganic Chemistry*, **2013**, 52, 3976-84	5.1	28
301	Understanding the Nature of the CH□□HC Interactions in Alkanes. *Journal of Chemical Theory and Computation*, **2013**, 9, 1977-91	6.4	90
300	A metal-metal bond in the light-induced state of [NiFe] hydrogenases with relevance to hydrogen evolution. *Journal of the American Chemical Society*, **2013**, 135, 3915-25	16.4	84

299	Derivation and assessment of relativistic hyperfine-coupling tensors on the basis of orbital-optimized second-order Møller-Plesset perturbation theory and the second-order Douglas-Kroll-Hess transformation. *Journal of Chemical Physics*, **2013**, 138, 104102	3.9	18
298	On the magnetic and spectroscopic properties of high-valent Mn3CaO4 cubanes as structural units of natural and artificial water-oxidizing catalysts. *Journal of the American Chemical Society*, **2013**, 135, 5726-39	16.4	81
297	Introduction to Ligand Field Theory **2013**, 23-51		2
296	Magnetic blocking in a linear iron(I) complex. *Nature Chemistry*, **2013**, 5, 577-81	17.6	486
295	A fully variational spin-orbit coupled complete active space self-consistent field approach: application to electron paramagnetic resonance g-tensors. *Journal of Chemical Physics*, **2013**, 138, 104113	3.9	82
294	A combined DFT and restricted open-shell configuration interaction method including spin-orbit coupling: application to transition metal L-edge X-ray absorption spectroscopy. *Journal of Chemical Physics*, **2013**, 138, 204101	3.9	173
293	Electronic structures of octahedral Ni(II) complexes with "click" derived triazole ligands: a combined structural, magnetometric, spectroscopic, and theoretical study. *Inorganic Chemistry*, **2013**, 52, 6880-92	5.1	68
292	Excited states of large open-shell molecules: an efficient, general, and spin-adapted approach based on a restricted open-shell ground state wave function. *Journal of Physical Chemistry A*, **2013**, 117, 3069-83	2.8	69
291	Mössbauer spectroscopy as a probe of magnetization dynamics in the linear iron(I) and iron(II) complexes [Fe(C(SiMe3)3)2](1-/0.). *Inorganic Chemistry*, **2013**, 52, 13123-31	5.1	85
290	What is the most efficient way to reach the canonical MP2 basis set limit?. *Molecular Physics*, **2013**, 111, 2653-2662	1.7	30
289	First principles calculations of the structure and V L-edge X-ray absorption spectra of V2O5 using local pair natural orbital coupled cluster theory and spin-orbit coupled configuration interaction approaches. *Physical Chemistry Chemical Physics*, **2013**, 15, 7260-76	3.6	111
288	Speeding up spin-component-scaled third-order pertubation theory with the chain of spheres approximation: the COSX-SCS-MP3 method. *Molecular Physics*, **2013**, 111, 1190-1195	1.7	35
287	Iron Azides with Cyclam-Derived Ligands: Are They Precursors for High-Valent Iron Nitrides in the Gas Phase?. *ChemPlusChem*, **2013**, 78, 1053-1057	2.8	6
286	Reply to Mouesca et al.: Electronic structure of the proximal [4Fe-3S] cluster of O2-tolerant [NiFe] hydrogenases. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, E2539	11.5	2
285	Control of electronic properties of triphenylene by substitution. *Organic Electronics*, **2012**, 13, 71-83	3.5	12
284	The photochemistry of [Fe(III)N3(cyclam-ac)]PF6 at 266 nm. *Chemistry - A European Journal*, **2012**, 18, 3043-55	4.8	28
283	A Reduced (β-Diketiminato)iron Complex with End-On and Side-On Nitriles: Strong Backbonding or Ligand Non-Innocence?. *European Journal of Inorganic Chemistry*, **2012**, 2012, 479-483	2.3	11
282	Azurin as a protein scaffold for a low-coordinate nonheme iron site with a small-molecule binding pocket. *Journal of the American Chemical Society*, **2012**, 134, 19746-57	16.4	28

281	Key hydride vibrational modes in [NiFe] hydrogenase model compounds studied by resonance Raman spectroscopy and density functional calculations. *Inorganic Chemistry*, **2012**, 51, 11787-97	5.1	31
280	Detailed QM/MM study of the Electron Paramagnetic Resonance Parameters of Nitrosyl Myoglobin. *Journal of Chemical Theory and Computation*, **2012**, 8, 563-74	6.4	22
279	Reversible C-C bond formation between redox-active pyridine ligands in iron complexes. *Journal of the American Chemical Society*, **2012**, 134, 20352-64	16.4	70
278	Efficient and automatic calculation of optical band shapes and resonance Raman spectra for larger molecules within the independent mode displaced harmonic oscillator model. *Journal of Chemical Physics*, **2012**, 137, 234107	3.9	88
277	Detection of the water-binding sites of the oxygen-evolving complex of Photosystem II using W-band 17O electron-electron double resonance-detected NMR spectroscopy. *Journal of the American Chemical Society*, **2012**, 134, 16619-34	16.4	223
276	Ultrafast primary processes of an iron-(III) azido complex in solution induced with 266 nm light. *Physical Chemistry Chemical Physics*, **2012**, 14, 6165-72	3.6	20
275	How Do Heavier Halide Ligands Affect the Signs and Magnitudes of the Zero-Field Splittings in Halogenonickel(II) Scorpionate Complexes? A Theoretical Investigation Coupled to Ligand-Field Analysis. *Journal of Chemical Theory and Computation*, **2012**, 8, 2344-51	6.4	44
274	Oxygen activation in extradiol catecholate dioxygenases a density functional study. *Chemical Science*, **2012**, 3, 1600	9.4	55
273	A functional [NiFe]-hydrogenase model compound that undergoes biologically relevant reversible thiolate protonation. *Journal of the American Chemical Society*, **2012**, 134, 20745-55	16.4	95
272	Magnetic circular dichroism spectrum of the molybdenum(V) complex [Mo(O)Cl3dppe]: C-term signs and intensities for multideterminant excited doublet states. *Inorganic Chemistry*, **2012**, 51, 5748-63	5.1	6
271	Two interconvertible structures that explain the spectroscopic properties of the oxygen-evolving complex of photosystem II in the S2 state. *Angewandte Chemie - International Edition*, **2012**, 51, 9935-40	16.4	293
270	One-electron contributions to the g-tensor for second-order Douglas-Kroll-Hess theory. *Journal of Chemical Physics*, **2012**, 137, 094102	3.9	47
269	Zwei ineinander umwandelbare Strukturen erklären die spektroskopischen Eigenschaften des Wasser oxidierenden Enzyms des Photosystems II im S2-Zustand. *Angewandte Chemie*, **2012**, 124, 10074-10079	3.6	25
268	Reactivity studies on [Cp?MnX(thf)]2: manganese amide and polyhydride synthesis. *Chemical Science*, **2012**, 3, 2972	9.4	23
267	Zero-field splitting in a series of structurally related mononuclear Ni(II)-bispidine complexes. *Inorganic Chemistry*, **2012**, 51, 12324-35	5.1	33
266	All-electron scalar relativistic basis sets for the 6p elements. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	79
265	Metal-to-metal charge-transfer transitions: reliable excitation energies from ab initio calculations. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	26
264	Outer-sphere contributions to the electronic structure of type zero copper proteins. *Journal of the American Chemical Society*, **2012**, 134, 8241-53	16.4	36

263	Computational study of the electronic structure and magnetic properties of the Ni-C state in [NiFe] hydrogenases including the second coordination sphere. *Journal of Biological Inorganic Chemistry*, **2012**, 17, 1269-81	3.7	42
262	Manganese K-edge X-ray absorption spectroscopy as a probe of the metal-ligand interactions in coordination compounds. *Inorganic Chemistry*, **2012**, 51, 680-7	5.1	91
261	Investigating magnetostructural correlations in the pseudooctahedral trans-[Ni(II){(OPPh2)(EPPh2)N}2(sol)2] complexes (E = S, Se; sol = DMF, THF) by magnetometry, HFEPR, and ab initio quantum chemistry. *Inorganic Chemistry*, **2012**, 51, 7218-31	5.1	35
260	ENDOR spectroscopy and DFT calculations: evidence for the hydrogen-bond network within R2 in the PCET of E. coli ribonucleotide reductase. *Journal of the American Chemical Society*, **2012**, 134, 17661-70	16.4	45
259	Electronic structure of nickel(II) and zinc(II) borohydrides from spectroscopic measurements and computational modeling. *Inorganic Chemistry*, **2012**, 51, 2793-805	5.1	26
258	The ORCA program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 73-78	7.9	6710
257	Improved correlation energy extrapolation schemes based on local pair natural orbital methods. *Journal of Physical Chemistry A*, **2012**, 116, 4801-16	2.8	88
256	An unusal case of facile non-degenerate P-C bond making and breaking. *Chemistry - an Asian Journal*, **2012**, 7, 1708-12	4.5	15
255	Electronic structure analysis of the oxygen-activation mechanism by Fe(II)- and α-ketoglutarate (αKG)-dependent dioxygenases. *Chemistry - A European Journal*, **2012**, 18, 6555-67	4.8	79
254	Deoxygenation of coordinated oxaphosphiranes: a new route to P=C double-bond systems. *Chemistry - A European Journal*, **2012**, 18, 9780-3	4.8	14
253	Synthesis, Chiral Resolution, and Absolute Configuration of Functionalized Tröger's Base Derivatives: Part II. *ChemPlusChem*, **2012**, 77, 396-403	2.8	24
252	Accurate thermochemistry from a parameterized coupled-cluster singles and doubles model and a local pair natural orbital based implementation for applications to larger systems. *Journal of Chemical Physics*, **2012**, 136, 064101	3.9	64
251	Reductive activation of the heme iron-nitrosyl intermediate in the reaction mechanism of cytochrome c nitrite reductase: a theoretical study. *Journal of Biological Inorganic Chemistry*, **2012**, 17, 741-60	3.7	34
250	The resolution of identity and chain of spheres approximations for the LPNO-CCSD singles Fock term. *Molecular Physics*, **2012**, 110, 2413-2417	1.7	29
249	Weak Molecular Interactions Studied with Parallel Implementations of the Local Pair Natural Orbital Coupled Pair and Coupled Cluster Methods. *Journal of Chemical Theory and Computation*, **2011**, 7, 76-87	6.4	127
248	Effect of Ca2+/Sr2+ substitution on the electronic structure of the oxygen-evolving complex of photosystem II: a combined multifrequency EPR, 55Mn-ENDOR, and DFT study of the S2 state. *Journal of the American Chemical Society*, **2011**, 133, 3635-48	16.4	190
247	Zero field splitting of the chalcogen diatomics using relativistic correlated wave-function methods. *Journal of Chemical Physics*, **2011**, 135, 114106	3.9	26
246	Dynamic hydrogen-bonding network in the distal pocket of the nitrosyl complex of Pseudomonas aeruginosa cd1 nitrite reductase. *Journal of the American Chemical Society*, **2011**, 133, 3043-55	16.4	28

245	Protein-ligand interaction energies with dispersion corrected density functional theory and high-level wave function based methods. *Journal of Physical Chemistry A*, **2011**, 115, 11210-20	2.8	73
244	Manganese K X-ray emission spectroscopy as a probe of metal-ligand interactions. *Inorganic Chemistry*, **2011**, 50, 8397-409	5.1	105
243	Theoretical evaluation of structural models of the S2 state in the oxygen evolving complex of Photosystem II: protonation states and magnetic interactions. *Journal of the American Chemical Society*, **2011**, 133, 19743-57	16.4	249
242	Efficient and accurate local single reference correlation methods for high-spin open-shell molecules using pair natural orbitals. *Journal of Chemical Physics*, **2011**, 135, 214102	3.9	146
241	Interplay of Correlation and Relativistic Effects in Correlated Calculations on Transition-Metal Complexes: The (Cu2O2)(2+) Core Revisited. *Journal of Chemical Theory and Computation*, **2011**, 7, 1511-23	5.4	85
240	Some Thoughts on the Scope of Linear Scaling Self-Consistent Field Electronic Structure Methods. *Challenges and Advances in Computational Chemistry and Physics*, **2011**, 227-261	0.7	6
239	Theoretical analysis of the spin Hamiltonian parameters in Co(II)S4 complexes, using density functional theory and correlated ab initio methods. *Inorganic Chemistry*, **2011**, 50, 8741-54	5.1	98
238	Electronic structures and spectroscopy of the electron transfer series [Fe(NO)L2]z (z = 1+, 0, 1-, 2-, 3-; L = dithiolene). *Inorganic Chemistry*, **2011**, 50, 12064-74	5.1	27
237	Experimental and computational investigation of thiolate alkylation in Ni(II) and Zn(II) complexes: role of the metal on the sulfur nucleophilicity. *Inorganic Chemistry*, **2011**, 50, 10047-55	5.1	21
236	Nonheme oxo-iron(IV) intermediates form an oxyl radical upon approaching the C-H bond activation transition state. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 1228-33	11.5	212
235	Theoretical insights into the magnetostructural correlations in Mn3-based single-molecule magnets. *Inorganic Chemistry*, **2011**, 50, 2112-24	5.1	21
234	Quantum Chemistry and M sbauer Spectroscopy **2011**, 137-199		14
233	Efficient time-dependent density functional theory approximations for hybrid density functionals: analytical gradients and parallelization. *Journal of Chemical Physics*, **2011**, 134, 054116	3.9	148
232	First Principles Approach to Spin-Hamiltonian Parameters **2011**, 295-326		3
231	Detailed ab initio first-principles study of the magnetic anisotropy in a family of trigonal pyramidal iron(II) pyrrolide complexes. *Inorganic Chemistry*, **2011**, 50, 7460-77	5.1	120
230	The electronic structures of the S(2) states of the oxygen-evolving complexes of photosystem II in plants and cyanobacteria in the presence and absence of methanol. *Biochimica Et Biophysica Acta - Bioenergetics*, **2011**, 1807, 829-40	4.6	75
229	Revisiting the Atomic Natural Orbital Approach for Basis Sets: Robust Systematic Basis Sets for Explicitly Correlated and Conventional Correlated ab initio Methods?. *Journal of Chemical Theory and Computation*, **2011**, 7, 33-43	6.4	195
228	What is not required to make a single molecule magnet. *Faraday Discussions*, **2011**, 148, 229-38; discussion 299-314	3.6	265

227	X-ray emission spectroscopy evidences a central carbon in the nitrogenase iron-molybdenum cofactor. *Science*, **2011**, 334, 974-7	33.3	659
226	A Modern First-Principles View on Ligand Field Theory Through the Eyes of Correlated Multireference Wavefunctions. *Structure and Bonding*, **2011**, 149-220	0.9	66
225	An overlap fitted chain of spheres exchange method. *Journal of Chemical Physics*, **2011**, 135, 144105	3.9	456
224	Theoretical determination of the zero-field splitting in copper acetate monohydrate. *Inorganic Chemistry*, **2011**, 50, 6229-36	5.1	78
223	Substrate binding and activation in the active site of cytochrome c nitrite reductase: a density functional study. *Journal of Biological Inorganic Chemistry*, **2011**, 16, 417-30	3.7	36
222	Correlated wavefunction methods in bioinorganic chemistry. *Journal of Biological Inorganic Chemistry*, **2011**, 16, 821-9	3.7	41
221	The reaction mechanism of Cytochrome P450 NO reductase: a detailed quantum mechanics/molecular mechanics study. *ChemPhysChem*, **2011**, 12, 3192-203	3.2	32
220	A Fully Delocalized Mixed-Valence Bis-(Thiolato) Dicopper Complex: A Structural and Functional Model of the Biological CuA Center. *Angewandte Chemie*, **2011**, 123, 5780-5784	3.6	10
219	A fully delocalized mixed-valence bis-(thiolato) dicopper complex: a structural and functional model of the biological CuA center. *Angewandte Chemie - International Edition*, **2011**, 50, 5662-6	16.4	44
218	All-Electron Scalar Relativistic Basis Sets for the Actinides. *Journal of Chemical Theory and Computation*, **2011**, 7, 677-684	6.4	187
217	Prediction of high-valent iron K-edge absorption spectra by time-dependent density functional theory. *Dalton Transactions*, **2011**, 40, 11070-9	4.3	84
216	Influence of mixed thiolate/thioether versus dithiolate coordination on the accessibility of the uncommon +I and +III oxidation states for the nickel ion: an experimental and computational study. *Inorganic Chemistry*, **2011**, 50, 3707-16	5.1	30
215	Electronic structure of a weakly antiferromagnetically coupled Mn(II)Mn(III) model relevant to manganese proteins: a combined EPR, 55Mn-ENDOR, and DFT study. *Inorganic Chemistry*, **2011**, 50, 8238-51	5.1	46
214	Effect of Ca2+/Sr2+Substitution on the Electronic Structure of the Oxygen-Evolving Complex of Photosystem II: A Combined Multifrequency EPR,55Mn-ENDOR, and DFT Study of the S2State. *Journal of the American Chemical Society*, **2011**, 133, 14149-14149	16.4	7
213	The relationship between double excitation amplitudes and Z vector components in some post-Hartree-Fock correlation methods. *Journal of Chemical Physics*, **2011**, 135, 064103	3.9	3
212	An orbital-invariant and strictly size extensive post-Hartree-Fock correlation functional. *Journal of Chemical Physics*, **2011**, 135, 084102	3.9	17
211	Spectroscopic and computational studies of an end-on bound superoxo-Cu(II) complex: geometric and electronic factors that determine the ground state. *Inorganic Chemistry*, **2010**, 49, 9450-9	5.1	81
210	Accurate modeling of spin-state energetics in spin-crossover systems with modern density functional theory. *Inorganic Chemistry*, **2010**, 49, 772-4	5.1	181

209	Probing valence orbital composition with iron Kbeta X-ray emission spectroscopy. *Journal of the American Chemical Society*, **2010**, 132, 9715-27	16.4	209
208	Calibration of scalar relativistic density functional theory for the calculation of sulfur K-edge X-ray absorption spectra. *Inorganic Chemistry*, **2010**, 49, 1849-53	5.1	83
207	Cryoreduction of the NO-adduct of taurine:alpha-ketoglutarate dioxygenase (TauD) yields an elusive {FeNO}(8) species. *Journal of the American Chemical Society*, **2010**, 132, 4739-51	16.4	57
206	Family of V(III)-tristhiolato complexes relevant to functional models of vanadium nitrogenase: synthesis and electronic structure investigations by means of high-frequency and -field electron paramagnetic resonance coupled to quantum chemical computations. *Inorganic Chemistry*, **2010**, 49, 977-88	5.1	52
205	Correlated ab initio spin densities for larger molecules: orbital-optimized spin-component-scaled MP2 method. *Journal of Physical Chemistry A*, **2010**, 114, 11768-81	2.8	71
204	Efficient Structure Optimization with Second-Order Many-Body Perturbation Theory: The RIJCOSX-MP2 Method. *Journal of Chemical Theory and Computation*, **2010**, 6, 2325-38	6.4	187
203	Multireference ab initio calculations of g tensors for trinuclear copper clusters in multicopper oxidases. *Journal of Physical Chemistry B*, **2010**, 114, 7692-702	3.4	40
202	Experimental and theoretical EPR study of Jahn-Teller-active [HIPTN(3)N]MoL complexes (L = N(2), CO, NH(3)). *Journal of the American Chemical Society*, **2010**, 132, 8645-56	16.4	50
201	The coupled electron pair approximation: variational formulation and spin adaptation. *Molecular Physics*, **2010**, 108, 2449-2458	1.7	30
200	The resolution of the identity approximation for calculations of spin-spin contribution to zero-field splitting parameters. *Journal of Chemical Physics*, **2010**, 132, 144111	3.9	44
199	A Local Pair Natural Orbital Coupled Cluster Study of Rh Catalyzed Asymmetric Olefin Hydrogenation. *Journal of Chemical Theory and Computation*, **2010**, 6, 3137-44	6.4	46
198	Magnetic circular dichroism spectroscopy on the Cr□antiferromagnetic ring. *Dalton Transactions*, **2010**, 39, 4999-5004	4.3	16
197	Unsymmetrical one-electron oxidized Ni(II)-bis(salicylidene) complexes: a protonation-induced shift of the oxidation site. *Chemical Communications*, **2010**, 46, 6765-7	5.8	32
196	Revisiting the nitrosyl complex of myoglobin by high-field pulse EPR spectroscopy and quantum mechanical calculations. *Physical Chemistry Chemical Physics*, **2010**, 12, 7276-89	3.6	35
195	Reversible apical coordination of imidazole between the Ni(III) and Ni(II) oxidation states of a dithiolate complex: a process related to the Ni superoxide dismutase. *Inorganic Chemistry*, **2010**, 49, 6399-401	5.1	33
194	Spin interaction in octahedral zinc complexes of mono- and diradical Schiff and mannich bases. *Inorganic Chemistry*, **2010**, 49, 646-58	5.1	43
193	Hydroquinoid Chromium Complexes Bearing an Acyclic Conjugated Bridge: Chromium-Templated Synthesis, Molecular Structure, and Haptotropic Metal Migration. *Organometallics*, **2010**, 29, 6172-6185	3.8	11
192	Activation of a water molecule using a mononuclear Mn complex: from Mn-aquo, to Mn-hydroxo, to Mn-oxyl charge compensation. *Energy and Environmental Science*, **2010**, 3, 924-938	35.4	49

191	Dealing with Complexity in Open-Shell Transition Metal Chemistry from a Theoretical Perspective: Reaction Pathways, Bonding, Spectroscopy, And Magnetic Properties. *Advances in Inorganic Chemistry*, **2010**, 62, 301-349	2.1	33
190	Tetrahedral and square planar Ni[(SPR(2))(2)N](2) complexes, R = Ph & (i)Pr revisited: experimental and theoretical analysis of interconversion pathways, structural preferences, and spin delocalization. *Inorganic Chemistry*, **2010**, 49, 5079-93	5.1	45
189	Theoretical magnetochemistry of dinuclear manganese complexes: broken symmetry density functional theory investigation on the influence of bridging motifs on structure and magnetism. *Dalton Transactions*, **2010**, 39, 4959-67	4.3	93
188	Systematic theoretical study of the zero-field splitting in coordination complexes of Mn(III). Density functional theory versus multireference wave function approaches. *Journal of Physical Chemistry A*, **2010**, 114, 10750-8	2.8	123
187	The unusual electronic structure of dinitrosyl iron complexes. *Journal of the American Chemical Society*, **2010**, 132, 3646-7	16.4	92
186	Understanding the Zero-Field Splitting of Mononuclear Manganese(II) Complexes from Combined EPR Spectroscopy and Quantum Chemistry. *Applied Magnetic Resonance*, **2010**, 37, 229-245	0.8	61
185	Calculation of Magnetic Tensors and EPR Spectra for Free Radicals in Different Environments **2010**, 63-104		5
184	3,4,5,6-Tetrafluorophenylnitren-2-yl: a ground-state quartet triradical. *Chemistry - A European Journal*, **2010**, 16, 4496-506	4.8	17
183	Analysis of Reaction Channels for Alkane Hydroxylation by Nonheme Iron(IV)Oxo Complexes. *Angewandte Chemie*, **2010**, 122, 5853-5856	3.6	41
182	Einblicke in die Chemie kurzlebiger P-Chlorphosphanyl-Komplexe. *Angewandte Chemie*, **2010**, 122, 7047-7051	3.6	11
181	X-ray structures of copper(II) and nickel(II) radical salen complexes: the preference of galactose oxidase for copper(II). *Angewandte Chemie - International Edition*, **2010**, 49, 4989-92	16.4	150
180	Analysis of reaction channels for alkane hydroxylation by nonheme iron(IV)-oxo complexes. *Angewandte Chemie - International Edition*, **2010**, 49, 5717-20	16.4	176
179	Insights into the chemistry of transient P-chlorophosphanyl complexes. *Angewandte Chemie - International Edition*, **2010**, 49, 6894-8	16.4	30
178	An unusual stable mononuclear Mn(III) bis-terpyridine complex exhibiting Jahn-Teller compression: electrochemical synthesis, physical characterisation and theoretical study. *Chemistry - A European Journal*, **2009**, 15, 980-8	4.8	55
177	The quest for ring opening of oxaphosphirane complexes: a coupled-cluster and density functional study of CH(3)PO isomers and their Cr(CO)(5) complexes. *Chemistry - A European Journal*, **2009**, 15, 2594-601	4.8	38
176	How to build molecules with large magnetic anisotropy. *Chemistry - A European Journal*, **2009**, 15, 4078-87	4.8	139
175	EPR spectroscopy of a family of Cr(III) 7M(II) (M = Cd, Zn, Mn, Ni) "wheels": studies of isostructural compounds with different spin ground states. *Chemistry - A European Journal*, **2009**, 15, 3152-67	4.8	70
174	A new quantum chemical approach to the magnetic properties of oligonuclear transition-metal complexes: application to a model for the tetranuclear manganese cluster of photosystem II. *Chemistry - A European Journal*, **2009**, 15, 5108-23	4.8	106

173	Magnetic circular dichroism spectroscopy of weakly exchange coupled transition metal dimers: A model study. *Coordination Chemistry Reviews*, **2009**, 253, 2352-2362	23.2	20
172	Density functional theory. *Photosynthesis Research*, **2009**, 102, 443-53	3.7	174
171	Quantum chemical studies of C-H activation reactions by high-valent nonheme iron centers. *Current Opinion in Chemical Biology*, **2009**, 13, 89-98	9.7	105
170	Prediction of molecular properties and molecular spectroscopy with density functional theory: From fundamental theory to exchange-coupling. *Coordination Chemistry Reviews*, **2009**, 253, 526-563	23.2	827
169	Efficient, approximate and parallel Hartree–Fock and hybrid DFT calculations. A 'chain-of-spheres' algorithm for the Hartree–Fock exchange. *Chemical Physics*, **2009**, 356, 98-109	2.3	1458
168	Comparison of two efficient approximate Hartree–Fock approaches. *Chemical Physics Letters*, **2009**, 481, 240-243	2.5	242
167	Magnetic and spectroscopic properties of mixed valence manganese(III,IV) dimers: a systematic study using broken symmetry density functional theory. *Inorganic Chemistry*, **2009**, 48, 7251-60	5.1	98
166	Trinuclear terpyridine frustrated spin system with a Mn(IV)3O4 core: synthesis, physical characterization, and quantum chemical modeling of its magnetic properties. *Inorganic Chemistry*, **2009**, 48, 10281-8	5.1	50
165	Spin-Hamiltonian Parameters from First Principle Calculations: Theory and Application. *Biological Magnetic Resonance*, **2009**, 175-229	0.5	19
164	Efficient and accurate local approximations to coupled-electron pair approaches: An attempt to revive the pair natural orbital method. *Journal of Chemical Physics*, **2009**, 130, 114108	3.9	419
163	Catalysis via homolytic substitutions with C-O and Ti-O bonds: oxidative additions and reductive eliminations in single electron steps. *Journal of the American Chemical Society*, **2009**, 131, 16989-99	16.4	100
162	A multiconfigurational ab initio study of the zero-field splitting in the di- and trivalent hexaquo-chromium complexes. *Inorganic Chemistry*, **2009**, 48, 10572-80	5.1	51
161	Iron(II) complexes with redox-active tetrazene (RNNNNR) ligands. *Inorganic Chemistry*, **2009**, 48, 4828-36	5.1	58
160	All-Electron Scalar Relativistic Basis Sets for the Lanthanides. *Journal of Chemical Theory and Computation*, **2009**, 5, 2229-38	6.4	227
159	A Comparative Study of a Triphenylene Tricarbonyl Chromium Complex and Its Uncoordinated Arene Ligand on the Ag(111) Surface: Influence of the Complexation on the Adsorption. *Journal of Physical Chemistry C*, **2009**, 113, 6014-6021	3.8	2
158	Calculation of electronic g-tensors using coupled cluster theory. *Journal of Physical Chemistry A*, **2009**, 113, 11541-9	2.8	50
157	Direct detection and characterization of chloride in the active site of the low-pH form of sulfite oxidase using electron spin echo envelope modulation spectroscopy, isotopic labeling, and density functional theory calculations. *Inorganic Chemistry*, **2009**, 48, 4743-52	5.1	31
156	Theoretical description of the structure and magnetic properties of nitroxide-Cu(II)-nitroxide spin triads by means of multiconfigurational ab initio calculations. *Journal of Physical Chemistry A*, **2009**, 113, 6149-57	2.8	49

155	Efficient and accurate approximations to the local coupled cluster singles doubles method using a truncated pair natural orbital basis. *Journal of Chemical Physics*, **2009**, 131, 064103	3.9	379
154	Assessment of Orbital-Optimized, Spin-Component Scaled Second-Order Many-Body Perturbation Theory for Thermochemistry and Kinetics. *Journal of Chemical Theory and Computation*, **2009**, 5, 3060-73	6.4	172
153	Interaction of radical pairs through-bond and through-space: scope and limitations of the point-dipole approximation in electron paramagnetic resonance spectroscopy. *Journal of the American Chemical Society*, **2009**, 131, 10092-106	16.4	99
152	Optical absorption and emission properties of rubrene: insight from a combined experimental and theoretical study. *New Journal of Physics*, **2009**, 11, 015001	2.9	96
151	Calibration of modern density functional theory methods for the prediction of 57Fe Mössbauer isomer shifts: meta-GGA and double-hybrid functionals. *Inorganic Chemistry*, **2009**, 48, 784-5	5.1	182
150	Multireference ab initio studies of zero-field splitting and magnetic circular dichroism spectra of tetrahedral Co(II) complexes. *Dalton Transactions*, **2009**, 6021-36	4.3	56
149	Accurate theoretical chemistry with coupled pair models. *Accounts of Chemical Research*, **2009**, 42, 641-8	24.3	160
148	Exchangeable oxygens in the vicinity of the molybdenum center of the high-pH form of sulfite oxidase and sulfite dehydrogenase. *Physical Chemistry Chemical Physics*, **2009**, 11, 6733-42	3.6	20
147	Structure of the oxygen-evolving complex of photosystem II: information on the S(2) state through quantum chemical calculation of its magnetic properties. *Physical Chemistry Chemical Physics*, **2009**, 11, 6788-98	3.6	114
146	Ab initio and coupled-perturbed density functional theory estimation of zero-field splittings in MnII transition metal complexes. *Journal of Physical Chemistry A*, **2008**, 112, 7976-83	2.8	70
145	Electronic structure and spectroscopy of "superoxidized" iron centers in model systems: theoretical and experimental trends. *Physical Chemistry Chemical Physics*, **2008**, 10, 4361-74	3.6	77
144	First-principles calculations of magnetic circular dichroism spectra. *Journal of Chemical Physics*, **2008**, 128, 114117	3.9	79
143	All-Electron Scalar Relativistic Basis Sets for Third-Row Transition Metal Atoms. *Journal of Chemical Theory and Computation*, **2008**, 4, 908-19	6.4	832
142	Spectroscopic and theoretical study of a mononuclear manganese(III) complex exhibiting a tetragonally compressed geometry. *Inorganic Chemistry*, **2008**, 47, 439-47	5.1	51
141	2,3,5,6-Tetrafluorophenylnitren-4-yl: electron paramagnetic resonance spectroscopic characterization of a quartet-ground-state nitreno radical. *Journal of the American Chemical Society*, **2008**, 130, 4396-403	16.4	33
140	Multireference ab initio quantum mechanics/molecular mechanics study on intermediates in the catalytic cycle of cytochrome P450(cam). *Journal of Physical Chemistry A*, **2008**, 112, 12904-10	2.8	42
139	Prediction of iron K-edge absorption spectra using time-dependent density functional theory. *Journal of Physical Chemistry A*, **2008**, 112, 12936-43	2.8	217
138	A systematic density functional study of the zero-field splitting in Mn(II) coordination compounds. *Inorganic Chemistry*, **2008**, 47, 134-42	5.1	116

137	Ab initio study of intriguing coordination complexes: a metal field theory picture. *Journal of Physical Chemistry A*, **2008**, 112, 12975-9	2.8	13
136	Focusing the view on nature's water-splitting catalyst. *Philosophical Transactions of the Royal Society B: Biological Sciences*, **2008**, 363, 1167-77; discussion 1177	5.8	57
135	Latest developments and applications of double-hybrid density functionals. *Chemistry Central Journal*, **2008**, 2,		78
134	Definition of magneto-structural correlations for the MnII ion. *Chemistry - A European Journal*, **2008**, 14, 6498-509	4.8	61
133	The electronic structure of iron corroles: a combined experimental and quantum chemical study. *Chemistry - A European Journal*, **2008**, 14, 10839-51	4.8	105
132	A comparative study of single reference correlation methods of the coupled-pair type. *Chemical Physics*, **2008**, 343, 217-230	2.3	90
131	Time-dependent density functional calculations of ligand K-edge X-ray absorption spectra. *Inorganica Chimica Acta*, **2008**, 361, 965-972	2.7	177
130	Geometries of Third-Row Transition-Metal Complexes from Density-Functional Theory. *Journal of Chemical Theory and Computation*, **2008**, 4, 1449-59	6.4	363
129	The Ligand-Field Paradigm **2008**, 411-445		4
128	Molecular and electronic structure of square-planar gold complexes containing two 1,2-Di(4-tert-butylphenyl)ethylene-1,2-dithiolato ligands: [Au(2L)2]1+/0/1-/2-. A combined experimental and computational study. *Inorganic Chemistry*, **2007**, 46, 1100-11	5.1	58
127	Spectroscopic and computational evaluation of the structure of the high-spin Fe(IV)-oxo intermediates in taurine: alpha-ketoglutarate dioxygenase from Escherichia coli and its His99Ala ligand variant. *Journal of the American Chemical Society*, **2007**, 129, 6168-79	16.4	167
126	Performance of modern density functional theory for the prediction of hyperfine structure: meta-GGA and double hybrid functionals. *Molecular Physics*, **2007**, 105, 2049-2071	1.7	110
125	Analytic derivative calculation of electronic g-tensors based on multireference configuration interaction wavefunctions. *Molecular Physics*, **2007**, 105, 2507-2514	1.7	37
124	Synthesis and spectroscopic characterization of copper(II)-nitrito complexes with hydrotris(pyrazolyl)borate and related coligands. *Inorganic Chemistry*, **2007**, 46, 3916-33	5.1	83
123	Characterization of a genuine iron(V)-nitrido species by nuclear resonant vibrational spectroscopy coupled to density functional calculations. *Journal of the American Chemical Society*, **2007**, 129, 11053-60	16.4	66
122	The catalytic Mn2+ sites in the enolase-inhibitor complex: crystallography, single-crystal EPR, and DFT calculations. *Journal of the American Chemical Society*, **2007**, 129, 4240-52	16.4	24
121	Analysis and prediction of absorption band shapes, fluorescence band shapes, resonance Raman intensities, and excitation profiles using the time-dependent theory of electronic spectroscopy. *Journal of Chemical Physics*, **2007**, 127, 164319	3.9	231
120	Description of the ground-state covalencies of the bis(dithiolato) transition-metal complexes from X-ray absorption spectroscopy and time-dependent density-functional calculations. *Chemistry - A European Journal*, **2007**, 13, 2783-97	4.8	181

119	Electronic structures of five-coordinate complexes of iron containing zero, one, or two pi-radical ligands: a broken-symmetry density functional theoretical study. *Chemistry - A European Journal*, **2007**, 13, 8390-403	4.8	32
118	Fragmentation of the (Cyclam-acetato)iron Azide Cation in the Gas Phase. *European Journal of Inorganic Chemistry*, **2007**, 2007, 816-821	2.3	31
117	Theoretical bioinorganic chemistry: the electronic structure makes a difference. *Current Opinion in Chemical Biology*, **2007**, 11, 134-41	9.7	122
116	Advanced aspects of ab initio theoretical optical spectroscopy of transition metal complexes: Multiplets, spin-orbit coupling and resonance Raman intensities. *Coordination Chemistry Reviews*, **2007**, 251, 288-327	23.2	253
115	Bis(alpha-diimine)nickel complexes: molecular and electronic structure of three members of the electron-transfer series [Ni(L)(2)](z)() (z = 0, 1+, 2+) (L = 2-Phenyl-1,4-bis(isopropyl)-1,4-diazabutadiene). A combined experimental and theoretical study. *Inorganic Chemistry*, **2007**, 46, 5327-37	5.1	108
114	Calculation of the zero-field splitting tensor on the basis of hybrid density functional and Hartree-Fock theory. *Journal of Chemical Physics*, **2007**, 127, 164112	3.9	310
113	First-principles calculation of nuclear resonance vibrational spectra. *Hyperfine Interactions*, **2007**, 175, 165-174	0.8	28
112	Insights into the nature of the hydrogen bonding of *Tyr272 in apo-galactose oxidase. *Journal of Inorganic Biochemistry*, **2007**, 101, 1859-64	4.2	9
111	Importance of the anisotropic exchange interaction for the magnetic anisotropy of polymetallic systems. *Journal of the American Chemical Society*, **2007**, 129, 760-1	16.4	57
110	Joint spectroscopic and theoretical investigations of transition metal complexes involving non-innocent ligands. *Dalton Transactions*, **2007**, 1552-66	4.3	272
109	Origin of the zero-field splitting in mononuclear octahedral dihalide MnII complexes: an investigation by multifrequency high-field electron paramagnetic resonance and density functional theory. *Inorganic Chemistry*, **2007**, 46, 4905-16	5.1	108
108	Double-hybrid density functional theory for excited electronic states of molecules. *Journal of Chemical Physics*, **2007**, 127, 154116	3.9	339
107	Analytic derivatives for perturbatively corrected "double hybrid" density functionals: theory, implementation, and applications. *Journal of Chemical Physics*, **2007**, 126, 124115	3.9	162
106	Theoretical Bioinorganic Spectroscopy **2006**, 47-83		13
105	QM/MM calculations with DFT for taking into account protein effects on the EPR and optical spectra of metalloproteins. Plastocyanin as a case study. *Journal of Computational Chemistry*, **2006**, 27, 1463-75	3.5	97
104	Der Yandulov-Schrock-Zyklus und die Nitrogenase-Reaktion: dichtefunktionaltheoretische Untersuchung der Stickstoff-Fixierung. *Angewandte Chemie*, **2006**, 118, 202-205	3.6	12
103	Electronic structure of binuclear mixed valence copper azacryptates derived from integrated advanced EPR and DFT calculations. *Journal of the American Chemical Society*, **2006**, 128, 2017-29	16.4	47
102	Molecular and electronic structures of tetrahedral complexes of nickel and cobalt containing N,N'-disubstituted, bulky o-diiminobenzosemiquinonate(1-) pi-radical ligands. *Inorganic Chemistry*, **2006**, 45, 6298-307	5.1	94

101	Multireference ab initio calculations on reaction intermediates of the multicopper oxidases. *Inorganic Chemistry*, **2006**, 45, 11051-9	5.1	39
100	Octahedral non-heme oxo and non-oxo Fe(IV) complexes: an experimental/theoretical comparison. *Journal of the American Chemical Society*, **2006**, 128, 13515-28	16.4	40
99	Vibrational markers for the open-shell character of transition metal bis-dithiolenes: an infrared, resonance raman, and quantum chemical study. *Journal of the American Chemical Society*, **2006**, 128, 4422-36	16.4	88
98	Molecular and electronic structures of oxo-bis(benzene-1,2-dithiolato)chromate(V) monoanions. A combined experimental and density functional study. *Inorganic Chemistry*, **2006**, 45, 3499-509	5.1	48
97	An octahedral coordination complex of iron(VI). *Science*, **2006**, 312, 1937-41	33.3	253
96	Electronic structure of mononuclear bis(1,2-diaryl-1,2-ethylenedithiolato)iron complexes containing a fifth cyanide or phosphite ligand: a combined experimental and computational study. *Inorganic Chemistry*, **2006**, 45, 7877-90	5.1	29
95	Effect of N-methylation of macrocyclic amine ligands on the spin state of iron(III): a tale of two fluoro complexes. *Inorganic Chemistry*, **2006**, 45, 2027-37	5.1	40
94	Calculation of solvent shifts on electronic g-tensors with the conductor-like screening model (COSMO) and its self-consistent generalization to real solvents (direct COSMO-RS). *Journal of Physical Chemistry A*, **2006**, 110, 2235-45	2.8	520
93	Theoretische Chemie 2005. *Nachrichten Aus Der Chemie*, **2006**, 54, 276-281	0.1	
92	Theoretical spectroscopy of model-nonheme [Fe(IV)OL5]2+ complexes in their lowest triplet and quintet states using multireference ab initio and density functional theory methods. *Journal of Inorganic Biochemistry*, **2006**, 100, 716-26	4.2	123
91	Importance of direct spin-spin coupling and spin-flip excitations for the zero-field splittings of transition metal complexes: a case study. *Journal of the American Chemical Society*, **2006**, 128, 10213-22	16.4	388
90	Electronic structure of bis(imino)pyridine iron dichloride, monochloride, and neutral ligand complexes: a combined structural, spectroscopic, and computational study. *Journal of the American Chemical Society*, **2006**, 128, 13901-12	16.4	425
89	First-principles calculations of zero-field splitting parameters. *Journal of Chemical Physics*, **2006**, 125, 24103	3.9	267
88	Spin-spin contributions to the zero-field splitting tensor in organic triplets, carbenes and biradicals-a density functional and ab initio study. *Journal of Physical Chemistry A*, **2006**, 110, 12267-75	2.8	165
87	A critical evaluation of DFT, including time-dependent DFT, applied to bioinorganic chemistry. *Journal of Biological Inorganic Chemistry*, **2006**, 11, 702-11	3.7	302
86	The Yandulov/Schrock cycle and the nitrogenase reaction: pathways of nitrogen fixation studied by density functional theory. *Angewandte Chemie - International Edition*, **2005**, 45, 196-9	16.4	56
85	The electronic structure of the isoelectronic, square-planar complexes [FeII(L)2]2- and [CoIII(L Bu)2]- (L2- and (L Bu)2-=benzene-1,2-dithiolates): an experimental and density functional theoretical study. *Journal of the American Chemical Society*, **2005**, 127, 4403-15	16.4	161
84	Calculating absorption shifts for retinal proteins: computational challenges. *Journal of Physical Chemistry B*, **2005**, 109, 3606-15	3.4	221

83	Efficient and accurate approximations to the molecular spin-orbit coupling operator and their use in molecular g-tensor calculations. *Journal of Chemical Physics*, **2005**, 122, 34107	3.9	481
82	Modulation of the electronic structure and the Ni-Fe distance in heterobimetallic models for the active site in [NiFe]hydrogenase. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 18280-5	11.5	150
81	Calculation of electric-field gradients based on higher-order generalized Douglas-Kroll transformations. *Journal of Chemical Physics*, **2005**, 122, 204107	3.9	80
80	Spectroscopy of non-heme iron thiolate complexes: insight into the electronic structure of the low-spin active site of nitrile hydratase. *Inorganic Chemistry*, **2005**, 44, 1826-36	5.1	35
79	Pulsed EPR investigations of systems modeling molybdenum enzymes: hyperfine and quadrupole parameters of oxo-17O in [Mo 17O(SPh)4]-. *Journal of the American Chemical Society*, **2005**, 127, 16713-22	16.4	46
78	Performance of nonrelativistic and quasi-relativistic hybrid DFT for the prediction of electric and magnetic hyperfine parameters in 57Fe Mössbauer spectra. *Inorganic Chemistry*, **2005**, 44, 2245-54	5.1	191
77	Spin density distribution in five- and six-coordinate iron(II)-porphyrin NO complexes evidenced by magnetic circular dichroism spectroscopy. *Inorganic Chemistry*, **2005**, 44, 2570-2	5.1	84
76	Toward identification of the compound I reactive intermediate in cytochrome P450 chemistry: a QM/MM study of its EPR and Mössbauer parameters. *Journal of the American Chemical Society*, **2005**, 127, 5840-53	16.4	240
75	Determination of the g-tensors and their orientations for cis,trans-(L-N2S2)Mo(V)OX (X = Cl, SCH2Ph) by single-crystal EPR spectroscopy and molecular orbital calculations. *Inorganic Chemistry*, **2005**, 44, 1290-301	5.1	34
74	NosX function connects to nitrous oxide (N2O) reduction by affecting the Cu(Z) center of NosZ and its activity in vivo. *FEBS Letters*, **2005**, 579, 4605-9	3.8	24
73	Electronic structure of square planar bis(benzene-1,2-dithiolato)metal complexes [M(L)(2)](z) (z = 2-, 1-, 0; M = Ni, Pd, Pt, Cu, Au): an experimental, density functional, and correlated ab initio study. *Inorganic Chemistry*, **2005**, 44, 5345-60	5.1	243
72	EPR experiments to elucidate the structure of the ready and unready states of the [NiFe] hydrogenase of Desulfovibrio vulgaris Miyazaki F. *Biochemical Society Transactions*, **2005**, 33, 7-11	5.1	43
71	Square planar vs tetrahedral coordination in diamagnetic complexes of nickel(II) containing two bidentate pi-radical monoanions. *Inorganic Chemistry*, **2005**, 44, 3636-56	5.1	107
70	The geometric and electronic structure of [(cyclam-acetato)Fe(N)]+: a genuine iron(v) species with a ground-state spin S = 1/2. *Angewandte Chemie - International Edition*, **2005**, 44, 2908-12	16.4	134
69	Phenoxyl radicals hydrogen-bonded to imidazolium: analogues of tyrosyl D. of photosystem II: high-field EPR and DFT studies. *Angewandte Chemie - International Edition*, **2005**, 44, 5314-7	16.4	71
68	The Geometric and Electronic Structure of [(cyclam-acetato)Fe(N)]+: A Genuine Iron(V) Species with a Ground-State Spin S=1/2. *Angewandte Chemie*, **2005**, 117, 2968-2972	3.6	37
67	Phenoxyl Radicals Hydrogen-Bonded to Imidazolium: Analogues of Tyrosyl D. of Photosystem II: High-Field EPR and DFT Studies. *Angewandte Chemie*, **2005**, 117, 5448-5451	3.6	13
66	Dimanganese catalase--spectroscopic parameters from broken-symmetry density functional theory of the superoxidized Mn(III)/Mn(IV) state. *Journal of Biological Inorganic Chemistry*, **2005**, 10, 231-8	3.7	59

65	Comparison of density functionals for energy and structural differences between the high- [5T2g:(t2g)4(eg)2] and low- [1A1g:(t2g)6(eg)0] spin states of iron(II) coordination compounds. II. More functionals and the hexaminoferrous cation, [Fe(NH3)6]2+. *Journal of Chemical Physics*, **2005**, 122, 44110	3.9	142
64	A vertebrate-type ferredoxin domain in the Na+-translocating NADH dehydrogenase from Vibrio cholerae. *Journal of Biological Chemistry*, **2005**, 280, 22560-3	5.4	6
63	NADH oxidation by the Na+-translocating NADH:quinone oxidoreductase from Vibrio cholerae: functional role of the NqrF subunit. *Journal of Biological Chemistry*, **2004**, 279, 21349-55	5.4	47
62	Sum-over-states based multireference ab initio calculation of EPR spin Hamiltonian parameters for transition metal complexes. A case study. *Magnetic Resonance in Chemistry*, **2004**, 42 Spec no, S187-98	2.1	66
61	Definition of corresponding orbitals and the diradical character in broken symmetry DFT calculations on spin coupled systems. *Journal of Physics and Chemistry of Solids*, **2004**, 65, 781-785	3.9	372
60	Nonoxovanadium(IV) and oxovanadium(V) complexes with mixed O, X, O-donor ligands (X = S, Se, P, or PO). *Inorganic Chemistry*, **2004**, 43, 7324-38	5.1	77
59	Zero-Field Splitting **2004**, 541-564		19
58	Hydrogen bond geometries from electron paramagnetic resonance and electron-nuclear double resonance parameters: density functional study of quinone radical anion-solvent interactions. *Journal of the American Chemical Society*, **2004**, 126, 3280-90	16.4	113
57	Carboxylate binding in copper histidine complexes in solution and in zeolite Y: X- and W-band pulsed EPR/ENDOR combined with DFT calculations. *Journal of the American Chemical Society*, **2004** , 126, 11733-45	16.4	67
56	Comparison of density functionals for energy and structural differences between the high- [5T2g: (t2g)4(eg)2] and low- [1A1g: (t2g)6(eg)0] spin states of the hexaquoferrous cation [Fe(H2O)6]2+. *Journal of Chemical Physics*, **2004**, 120, 9473-86	3.9	161
55	Structural, spectroscopic, and computational study of an octahedral, non-heme [Fe-NO](6-8) Series: [Fe(NO)(cyclam-ac)]2+/+/0. *Journal of the American Chemical Society*, **2004**, 126, 5138-53	16.4	183
54	Electronic structure of the cysteine thiyl radical: a DFT and correlated ab initio study. *Journal of the American Chemical Society*, **2004**, 126, 2237-46	16.4	46
53	Calculating the electron paramagnetic resonance parameters of exchange coupled transition metal complexes using broken symmetry density functional theory: application to a MnIII/MnIV model compound. *Journal of the American Chemical Society*, **2004**, 126, 2613-22	16.4	176
52	Applications to EPR in Bioinorganic Chemistry **2004**, 581-591		7
51	Historical Aspects of EPR Parameter Calculations **2004**, 21-32		15
50	Molecular and electronic structure of four- and five-coordinate cobalt complexes containing two o-phenylenediamine- or two o-aminophenol-type ligands at various oxidation levels: an experimental, density functional, and correlated ab initio study. *Chemistry - A European Journal*,	4.8	196
49	Variable-Temperature Variable-Field Magnetic Circular Dichroism Combined with Electron Paramagnetic Resonance: Polarizations of Electronic Transitions in Solution. *ACS Symposium Series*, **2003**, 328-339	0.4	
48	Analysis and interpretation of metal-radical coupling in a series of square planar nickel complexes: correlated Ab initio and density functional investigation of [Ni(L(ISQ))(2)] (L(ISQ)=3,5-di-tert-butyl-o-diiminobenzosemiquinonate(1-)). *Journal of the American Chemical Society*, **2003**, 125, 10997-11005	16.4	264

47	An improvement of the resolution of the identity approximation for the formation of the Coulomb matrix. *Journal of Computational Chemistry*, **2003**, 24, 1740-7	3.5	614
46	Bioanorganische Reaktionsmechanismen: von hochvalenten Eisenzentren zur Bioorganometallchemie. *Angewandte Chemie*, **2003**, 115, 3048-3051	3.6	6
45	Bioinorganic reaction mechanisms: from high-valent iron to bioorganometallic chemistry. *Angewandte Chemie - International Edition*, **2003**, 42, 2942-5	16.4	20
44	Correlated ab initio calculation of electronic g-tensors using a sum over states formulation. *Chemical Physics Letters*, **2003**, 380, 721-728	2.5	34
43	Quantum chemical calculations of spectroscopic properties of metalloproteins and model compounds: EPR and Mössbauer properties. *Current Opinion in Chemical Biology*, **2003**, 7, 125-35	9.7	139
42	Molecular and electronic structures of bis-(o-diiminobenzosemiquinonato)metal(II) complexes (Ni, Pd, Pt), their monocations and -anions, and of dimeric dications containing weak metal-metal bonds. *Journal of the American Chemical Society*, **2003**, 125, 9116-28	16.4	209
41	A spectroscopy oriented configuration interaction procedure. *Journal of Chemical Physics*, **2003**, 119, 9428-9443	3.9	333
40	Noninnocence of the ligand glyoxal-bis(2-mercaptoanil). The electronic structures of [Fe(gma)]2, [Fe(gma)(py)] x py, [Fe(gma)(CN)]1-/0, [Fe(gma)I], and [Fe(gma)(PR3)(n)] (n = 1, 2). Experimental and theoretical evidence for "excited state" coordination. *Journal of the American Chemical Society*, **2003**, 125, 1293-308	16.4	87
39	Mixed-valent [FeIV(mu-O)(mu-carboxylato)2FeIII]3+ core. *Journal of the American Chemical Society*, **2003**, 125, 15554-70	16.4	75
38	Metal and ligand hyperfine couplings in transition metal complexes: The effect of spin–orbit coupling as studied by coupled perturbed Kohn–Sham theory. *Journal of Chemical Physics*, **2003**, 118, 3939-3948	3.9	324
37	Inactivation of the Na+-translocating NADH:ubiquinone oxidoreductase from Vibrio alginolyticus by reactive oxygen species. *FEBS Journal*, **2002**, 269, 1287-92		6
36	Prediction and interpretation of the 57Fe isomer shift in Mössbauer spectra by density functional theory. *Inorganica Chimica Acta*, **2002**, 337, 181-192	2.7	472
35	Efficient use of the resolution of the identity approximation in time-dependent density functional calculations with hybrid density functionals. *Chemical Physics Letters*, **2002**, 362, 170-178	2.5	161
34	Pentahaem cytochrome c nitrite reductase: reaction with hydroxylamine, a potential reaction intermediate and substrate. *Biochemical Society Transactions*, **2002**, 30, 649-53	5.1	27
33	o-Iminobenzosemiquinonato(1-) and o-amidophenolato(2-) complexes of palladium(II) and platinum(II): a combined experimental and density functional theoretical study. *Inorganic Chemistry*, **2002**, 41, 4295-303	5.1	117
32	Mechanism of the six-electron reduction of nitrite to ammonia by cytochrome c nitrite reductase. *Journal of the American Chemical Society*, **2002**, 124, 11737-45	16.4	256
31	Tuning the electronic structure of octahedral iron complexes [FeL(X)] (L = 1-alkyl-4,7-bis(4-tert-butyl-2-mercaptobenzyl)-1,4,7-triazacyclononane, X = Cl, CH(3)O, CN, NO). The S = 1/2 3/2 Spin equilibrium of [FeL(Pr)(NO)]. *Inorganic Chemistry*, **2002**, 41, 3444-56	5.1	100
30	Theoretical evidence for the singlet diradical character of square planar nickel complexes containing two o-semiquinonato type ligands. *Inorganic Chemistry*, **2002**, 41, 4179-93	5.1	284

29	Spectroscopic and electronic structure studies of protocatechuate 3,4-dioxygenase: nature of tyrosinate-Fe(III) bonds and their contribution to reactivity. *Journal of the American Chemical Society*, **2002**, 124, 602-14	16.4	80
28	Electron-mediating Cu(A) centers in proteins: a comparative high field (1)H ENDOR study. *Journal of the American Chemical Society*, **2002**, 124, 8152-62	16.4	34
27	Electronic structure and reactivity of low-spin Fe(III)-hydroperoxo complexes: comparison to activated bleomycin. *Journal of the American Chemical Society*, **2002**, 124, 10810-22	16.4	112
26	Configuration interaction calculation of electronic g tensors in transition metal complexes*. *International Journal of Quantum Chemistry*, **2001**, 83, 104-114	2.1	67
25	Prediction of electron paramagnetic resonance g values using coupled perturbed Hartree□Fock and Kohn□Sham theory. *Journal of Chemical Physics*, **2001**, 115, 11080-11096	3.9	495
24	Molecular and electronic structure of [Mn(V)N(cyclam-acetato)]PF6. A combined experimental and DFT study. *Inorganic Chemistry*, **2001**, 40, 4191-8	5.1	19
23	Theoretical Study of Ligand Superhyperfine Structure. Application to Cu(II) Complexes. *Journal of Physical Chemistry A*, **2001**, 105, 4290-4299	2.8	120
22	Approximate second-order SCF convergence for spin unrestricted wavefunctions. *Chemical Physics Letters*, **2000**, 325, 93-98	2.5	33
21	Structural investigations of the CuA centre of nitrous oxide reductase from Pseudomonas stutzeri by site-directed mutagenesis and X-ray absorption spectroscopy. *FEBS Journal*, **2000**, 267, 1368-81		42
20	Geometric and electronic structure/function correlations in non-heme iron enzymes. *Chemical Reviews*, **2000**, 100, 235-350	68.1	1454
19	Electronic Structure of Activated Bleomycin: Oxygen Intermediates in Heme versus Non-Heme Iron. *Journal of the American Chemical Society*, **2000**, 122, 11703-11724	16.4	137
18	Relationship between the Dipole Strength of Ligand Pre-Edge Transitions and Metal-Ligand Covalency. *Inorganic Chemistry*, **1999**, 38, 4854-4860	5.1	70
17	MCD C-Term Signs, Saturation Behavior, and Determination of Band Polarizations in Randomly Oriented Systems with Spin S >/= (1)/(2). Applications to S = (1)/(2) and S = (5)/(2). *Inorganic Chemistry*, **1999**, 38, 1847-1865	5.1	204
16	Calculation of Zero-Field Splittings, g-Values, and the Relativistic Nephelauxetic Effect in Transition Metal Complexes. Application to High-Spin Ferric Complexes. *Inorganic Chemistry*, **1998**, 37, 6568-6582	5.1	268
15	Probing the ground state of the purple mixed valence CuA center in nitrous oxide reductase: a CW ENDOR (X-band) study of the 65Cu, 15N-histidine labeled enzyme and interpretation of hyperfine couplings by molecular orbital calculations. *Journal of Biological Inorganic Chemistry*, **1998**, 3, 53-67	3.7	8
14	Detailed Spectroscopic and Theoretical Studies on [Fe(EDTA)(O2)]3-:□Electronic Structure of the Side-on Ferric□Peroxide Bond and Its Relevance to Reactivity. *Journal of the American Chemical Society*, **1998**, 120, 12829-12848	16.4	139
13	Probing the ground state of the purple mixed valence Cu. *Journal of Biological Inorganic Chemistry*, **1998**, 3, 53	3.7	22
12	The electronic structure of the mixed-valence copper dimer [Cu2{N(CH2CH2NCHCHNCH2CH2)3N}]3+□*Journal of the Chemical Society Dalton Transactions*, **1997**, 4083-4088		12

11	New insights from spectroscopy into the structure/function relationships of lipoxygenases. *Chemistry and Biology*, **1997**, 4, 795-808		82
10	The Purple Mixed-Valence CuA Center in Nitrous-oxide Reductase: EPR of the Copper-63-, Copper-65-, and Both Copper-65- and [15N]Histidine-Enriched Enzyme and a Molecular Orbital Interpretation. *Journal of the American Chemical Society*, **1996**, 118, 8692-8699	16.4	145
9	The Electronic Structure of CuA: A Novel Mixed-Valence Dinuclear Copper Electron-Transfer Center. *Journal of the American Chemical Society*, **1996**, 118, 11501-11514	16.4	160
8	Reactions of nitric oxide with nitronyl nitroxides and oxygen: prediction of nitrite and nitrate formation by kinetic simulation. *Free Radical Research*, **1995**, 22, 47-56	4	66
7	Trapping of nitric oxide formed during photolysis of sodium nitroprusside in aqueous and lipid phases: an electron spin resonance study. *Photochemistry and Photobiology*, **1995**, 61, 325-30	3.6	43
6	The EPR-Detectable Copper of Nitrous Oxide Reductase as a Model for CuA in Cytochrome c Oxidase: A Multifrequency Electron Paramagnetic Resonance Investigation **1993**, 419-426		4
5	Chapter 4:Quantum Chemical Approaches to Spin-Hamiltonian Parameters. *Electron Paramagnetic Resonance*,73-95	1	13
4	A perturbative approach to multireference equation-of-motion coupled cluster. *Molecular Physics*,e1939185	1.7	3
3	An excited state coupled-cluster study on indigo dyes. *Molecular Physics*,e1965235	1.7	0
2	Interpretation and Calculation of Spin-Hamiltonian Parameters in Transition Metal Complexes345-466		39
1	Software update: The ORCA program system—Version 5.0. *Wiley Interdisciplinary Reviews: Computational Molecular Science*,	7.9	73