Frank Neese

List of Publications by Citations

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	The ORCA program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 73-78	7.9	6710
603	Software update: the ORCA program system, version 4.0. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1327	7.9	2068
602	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
601	Geometric and electronic structure/function correlations in non-heme iron enzymes. *Chemical Reviews*, **2000**, 100, 235-350	68.1	1454
600	An efficient and near linear scaling pair natural orbital based local coupled cluster method. *Journal of Chemical Physics*, **2013**, 138, 034106	3.9	890
599	Natural triple excitations in local coupled cluster calculations with pair natural orbitals. *Journal of Chemical Physics*, **2013**, 139, 134101	3.9	876
598	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
597	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
596	X-ray emission spectroscopy evidences a central carbon in the nitrogenase iron-molybdenum cofactor. *Science*, **2011**, 334, 974-7	33.3	659
595	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
594	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
593	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
592	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
591	Magnetic blocking in a linear iron(I) complex. *Nature Chemistry*, **2013**, 5, 577-81	17.6	486
590	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
589	The ORCA quantum chemistry program package. *Journal of Chemical Physics*, **2020**, 152, 224108	3.9	479
588	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

587	An overlap fitted chain of spheres exchange method. *Journal of Chemical Physics*, **2011**, 135, 144105	3.9	456
586	Slow magnetization dynamics in a series of two-coordinate iron(II) complexes. *Chemical Science*, **2013**, 4, 125-138	9.4	455
585	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
584	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
583	Biological water oxidation. *Accounts of Chemical Research*, **2013**, 46, 1588-96	24.3	407
582	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
581	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
580	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
579	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
578	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
577	Geometries of Third-Row Transition-Metal Complexes from Density-Functional Theory. *Journal of Chemical Theory and Computation*, **2008**, 4, 1449-59	6.4	363
576	Double-hybrid density functional theory for excited electronic states of molecules. *Journal of Chemical Physics*, **2007**, 127, 154116	3.9	339
575	A spectroscopy oriented configuration interaction procedure. *Journal of Chemical Physics*, **2003**, 119, 9428-9443	3.9	333
574	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
573	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
572	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
571	A four-coordinate cobalt(II) single-ion magnet with coercivity and a very high energy barrier. *Nature Communications*, **2016**, 7, 10467	17.4	295
570	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

569	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
568	Joint spectroscopic and theoretical investigations of transition metal complexes involving non-innocent ligands. *Dalton Transactions*, **2007**, 1552-66	4.3	272
567	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
566	First-principles calculations of zero-field splitting parameters. *Journal of Chemical Physics*, **2006**, 125, 24103	3.9	267
565	What is not required to make a single molecule magnet. *Faraday Discussions*, **2011**, 148, 229-38; discussion 299-314	3.6	265
564	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
563	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
562	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
561	An octahedral coordination complex of iron(VI). *Science*, **2006**, 312, 1937-41	33.3	253
560	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
559	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
558	Comparison of two efficient approximate Hartee–Fock approaches. *Chemical Physics Letters*, **2009**, 481, 240-243	2.5	242
557	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
556	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
555	All-Electron Scalar Relativistic Basis Sets for the Lanthanides. *Journal of Chemical Theory and Computation*, **2009**, 5, 2229-38	6.4	227
554	Metal oxidation states in biological water splitting. *Chemical Science*, **2015**, 6, 1676-1695	9.4	225
553	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
552	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

551	Calculating absorption shifts for retinal proteins: computational challenges. *Journal of Physical Chemistry B*, **2005**, 109, 3606-15	3.4	221
550	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
549	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
548	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
547	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
546	Probing valence orbital composition with iron Kbeta X-ray emission spectroscopy. *Journal of the American Chemical Society*, **2010**, 132, 9715-27	16.4	209
545	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
544	Automatic Generation of Auxiliary Basis Sets. *Journal of Chemical Theory and Computation*, **2017**, 13, 554-562	6.4	205
543	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
542	Low-energy spectrum of iron-sulfur clusters directly from many-particle quantum mechanics. *Nature Chemistry*, **2014**, 6, 927-33	17.6	197
541	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*, **2004**, 11, 204-24	4.8	196
540	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
539	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
538	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
537	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
536	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
535	All-Electron Scalar Relativistic Basis Sets for the Actinides. *Journal of Chemical Theory and Computation*, **2011**, 7, 677-684	6.4	187
534	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

533	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
532	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
531	Accurate modeling of spin-state energetics in spin-crossover systems with modern density functional theory. *Inorganic Chemistry*, **2010**, 49, 772-4	5.1	181
530	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
529	Time-dependent density functional calculations of ligand K-edge X-ray absorption spectra. *Inorganica Chimica Acta*, **2008**, 361, 965-972	2.7	177
528	Analysis of reaction channels for alkane hydroxylation by nonheme iron(IV)-oxo complexes. *Angewandte Chemie - International Edition*, **2010**, 49, 5717-20	16.4	176
527	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
526	Density functional theory. *Photosynthesis Research*, **2009**, 102, 443-53	3.7	174
525	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
524	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
523	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
522	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
521	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
520	A linear cobalt(II) complex with maximal orbital angular momentum from a non-Aufbau ground state. *Science*, **2018**, 362,	33.3	164
519	Analytic derivatives for perturbatively corrected "double hybrid" density functionals: theory, implementation, and applications. *Journal of Chemical Physics*, **2007**, 126, 124115	3.9	162
518	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
517	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
516	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

515	Accurate theoretical chemistry with coupled pair models. *Accounts of Chemical Research*, **2009**, 42, 641-8	24.3	160
514	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
513	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
512	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
511	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
510	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
509	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
508	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
507	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
506	How to build molecules with large magnetic anisotropy. *Chemistry - A European Journal*, **2009**, 15, 4078-87	4.8	139
505	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
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503	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
502	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
501	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
500	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
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498	Ammonia binding to the oxygen-evolving complex of photosystem II identifies the solvent-exchangeable oxygen bridge (μ-oxo) of the manganese tetramer. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 15561-6	11.5	130

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496	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
495	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
494	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
493	Theoretical bioinorganic chemistry: the electronic structure makes a difference. *Current Opinion in Chemical Biology*, **2007**, 11, 134-41	9.7	122
492	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
491	Theoretical Study of Ligand Superhyperfine Structure. Application to Cu(II) Complexes. *Journal of Physical Chemistry A*, **2001**, 105, 4290-4299	2.8	120
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489	A systematic density functional study of the zero-field splitting in Mn(II) coordination compounds. *Inorganic Chemistry*, **2008**, 47, 134-42	5.1	116
488	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
487	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
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485	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
484	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
483	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
482	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
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478	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
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476	Manganese KβX-ray emission spectroscopy as a probe of metal-ligand interactions. *Inorganic Chemistry*, **2011**, 50, 8397-409	5.1	105
475	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
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472	Chemical applications carried out by local pair natural orbital based coupled-cluster methods. *Chemical Society Reviews*, **2014**, 43, 5032-41	58.5	102
471	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
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469	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
468	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
467	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
466	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
465	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
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463	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
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