Frank Neese

List of Publications by Year
in descending order

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636 papers	81,838 citations	455 127 h-index	505 262 g-index
676 all docs	676 docs citations	676 times ranked	34185 citing authors

#	Article	IF	Citations
1	The ORCA program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 73-78.	16.2	9,659
2	Software update: the ORCA program system, version 4.0. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1327.	16.2	4,014
3	The ORCA quantum chemistry program package. Journal of Chemical Physics, 2020, 152, 224108.	2.9	2,387
4	Efficient, approximate and parallel Hartreeâ€“Fock and hybrid DFT calculations. A â€˜chain-of-spheresâ€™ algorithm for the Hartreeâ€“Fock exchange. Chemical Physics, 2009, 356, 98-109.	2.0	2,141
5	Geometric and Electronic Structure/Function Correlations in Non-Heme Iron Enzymes. Chemical Reviews, 2000, 100, 235-350.	49.4	1,615
6	Software update: The <scp>ORCA</scp> program systemâ€”Version 5.0. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	16.2	1,416
7	An efficient and near linear scaling pair natural orbital based local coupled cluster method. Journal of Chemical Physics, 2013, 138, 034106.	2.9	1,351
8	Natural triple excitations in local coupled cluster calculations with pair natural orbitals. Journal of Chemical Physics, 2013, 139, 134101.	2.9	1,309
9	All-Electron Scalar Relativistic Basis Sets for Third-Row Transition Metal Atoms. Journal of Chemical Theory and Computation, 2008, 4, 908-919.	5.4	1,124
10	Prediction of molecular properties and molecular spectroscopy with density functional theory: From fundamental theory to exchange-coupling. Coordination Chemistry Reviews, 2009, 253, 526-563.	19.2	943
11	An improvement of the resolution of the identity approximation for the formation of the Coulomb matrix. Journal of Computational Chemistry, 2003, 24, 1740-1747.	3.4	854
12	Sparse mapsâ€”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.	2.9	793
13	An overlap fitted chain of spheres exchange method. Journal of Chemical Physics, 2011, 135, 144105.	2.9	661
14	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, 034107.	2.9	636
15	Calculation of Solvent Shifts on Electronicg-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, 2235-2245.	2.5	582
16	Magnetic blocking in a linear iron(I) complex. Nature Chemistry, 2013, 5, 577-581.	13.7	582
17	Exploring the Accuracy Limits of Local Pair Natural Orbital Coupled-Cluster Theory. Journal of Chemical Theory and Computation, 2015, 11, 1525-1539.	5.4	570
18	Prediction and interpretation of the 57Fe isomer shift in MÃ¶ssbauer spectra by density functional theory. Inorganica Chimica Acta, 2002, 337, 181-192.	2.5	563

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19	Prediction of electron paramagnetic resonance g values using coupled perturbed Hartreeâ€“Fock and Kohnâ€“Sham theory. Journal of Chemical Physics, 2001, 115, 11080-11096.	2.9	547
20	Slow magnetization dynamics in a series of two-coordinate iron(<scp>ii</scp>) complexes. Chemical Science, 2013, 4, 125-138.	7.5	529
21	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.	2.9	499
22	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.	2.9	486
23	Importance of Direct Spinâ^'Spin Coupling and Spin-Flip Excitations for the Zero-Field Splittings of Transition Metal Complexes:Â A Case Study. Journal of the American Chemical Society, 2006, 128, 10213-10222.	14.1	463
24	Electronic Structure of Bis(imino)pyridine Iron Dichloride, Monochloride, and Neutral Ligand Complexes:Â A Combined Structural, Spectroscopic, and Computational Study. Journal of the American Chemical Society, 2006, 128, 13901-13912.	14.1	463
25	Biological Water Oxidation. Accounts of Chemical Research, 2013, 46, 1588-1596.	15.7	462
26	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.	2.9	454
27	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.	4.0	447
28	Geometries of Third-Row Transition-Metal Complexes from Density-Functional Theory. Journal of Chemical Theory and Computation, 2008, 4, 1449-1459.	5.4	431
29	Double-hybrid density functional theory for excited electronic states of molecules. Journal of Chemical Physics, 2007, 127, 154116.	2.9	416
30	A four-coordinate cobalt(II) single-ion magnet with coercivity and a very high energy barrier. Nature Communications, 2016, 7, 10467.	12.8	388
31	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.	2.9	361
32	A spectroscopy oriented configuration interaction procedure. Journal of Chemical Physics, 2003, 119, 9428-9443.	2.9	360
33	Metal and ligand hyperfine couplings in transition metal complexes: The effect of spinâ€“orbit coupling as studied by coupled perturbed Kohnâ€“Sham theory. Journal of Chemical Physics, 2003, 118, 3939-3948.	2.9	359
34	Two Interconvertible Structures that Explain the Spectroscopic Properties of the Oxygenâ€Evolving Complex of Photosystemâ€…II in the S₂ State. Angewandte Chemie - International Edition, 2012, 51, 9935-9940.	14.2	357
35	A critical evaluation of DFT, including time-dependent DFT, applied to bioinorganic chemistry. Journal of Biological Inorganic Chemistry, 2006, 11, 702-711.	2.7	341
36	First-principles calculations of zero-field splitting parameters. Journal of Chemical Physics, 2006, 125, 024103.	2.9	334

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37	What is not required to make a single molecule magnet. Faraday Discussions, 2011, 148, 229-238.	3.6	321
38	Comparison of two efficient approximate Harteeâ€“Fock approaches. Chemical Physics Letters, 2009, 481, 240-243.	2.6	317
39	Calculation of Zero-Field Splittings, g-Values, and the Relativistic Nephelauxetic Effect in Transition Metal Complexes. Application to High-Spin Ferric Complexesâ€. Inorganic Chemistry, 1998, 37, 6568-6582.	4.1	315
40	Theoretical Evidence for the Singlet Diradical Character of Square Planar Nickel Complexes Containing Two o-Semiquinonato Type Ligands. Inorganic Chemistry, 2002, 41, 4179-4193.	4.1	314
41	All-Electron Scalar Relativistic Basis Sets for the Lanthanides. Journal of Chemical Theory and Computation, 2009, 5, 2229-2238.	5.4	313
42	Mechanism of the Six-Electron Reduction of Nitrite to Ammonia by CytochromecNitrite Reductase. Journal of the American Chemical Society, 2002, 124, 11737-11745.	14.1	304
43	Joint spectroscopic and theoretical investigations of transition metal complexes involving non-innocent ligands. Dalton Transactions, 2007, , 1552.	3.3	304
44	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.	2.9	304
45	Analysis and Interpretation of Metal-Radical Coupling in a Series of Square Planar Nickel Complexes:Â Correlated Ab Initio and Density Functional Investigation of [Ni(LISQ)2] (LISQ=3,5-di-tert-butyl-o-diiminobenzosemiquinonate(1-)). Journal of the American Chemical Society, 2003, 125, 10997-11005.	14.1	300
46	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.	19.2	295
47	An Octahedral Coordination Complex of Iron(VI). Science, 2006, 312, 1937-1941.	19.6	294
48	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.	5.4	292
49	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.	19.2	286
50	Metal oxidation states in biological water splitting. Chemical Science, 2015, 6, 1676-1695.	7.5	283
51	All-Electron Scalar Relativistic Basis Sets for the Actinides. Journal of Chemical Theory and Computation, 2011, 7, 677-684.	5.4	282
52	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, 19743-19757.	14.1	275
53	A linear cobalt(II) complex with maximal orbital angular momentum from a non-Aufbau ground state. Science, 2018, 362, .	19.6	275
54	Electronic Structure of Square Planar Bis(benzene-1,2-dithiolato)metal Complexes [M(L)2]z(z= 2â^', 1â^',) Tj ETQq0 0 0 rgBT /Overlock 1 Chemistry, 2005, 44, 5345-5360.	4.1	269

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55	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.	2.9	265
56	Prediction of Iron K-Edge Absorption Spectra Using Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2008, 112, 12936-12943.	2.5	262
57	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, 4054-4063.	5.4	261
58	Toward Identification of the Compound I Reactive Intermediate in Cytochrome P450 Chemistry:â€‰ A QM/MM Study of Its EPR and MÃ¶ssbauer Parameters. Journal of the American Chemical Society, 2005, 127, 5840-5853.	14.1	253
59	Probing Valence Orbital Composition with Iron KÎ² X-ray Emission Spectroscopy. Journal of the American Chemical Society, 2010, 132, 9715-9727.	14.1	252
60	A theoretical analysis of chemical bonding, vibronic coupling, and magnetic anisotropy in linear iron(<scp>ii</scp>) complexes with single-molecule magnet behavior. Chemical Science, 2013, 4, 139-156.	7.5	251
61	Detection of the Water-Binding Sites of the Oxygen-Evolving Complex of Photosystem II Using W-Band¹⁷O Electronâ€“Electron Double Resonance-Detected NMR Spectroscopy. Journal of the American Chemical Society, 2012, 134, 16619-16634.	14.1	249
62	Low-energy spectrum of ironâ€“sulfur clusters directly from many-particle quantum mechanics. Nature Chemistry, 2014, 6, 927-933.	13.7	247
63	Efficient Structure Optimization with Second-Order Many-Body Perturbation Theory: The RIJCOSX-MP2 Method. Journal of Chemical Theory and Computation, 2010, 6, 2325-2338.	5.4	244
64	Nonheme oxo-iron(IV) intermediates form an oxyl radical upon approaching the Câ€“H bond activation transition state. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 1228-1233.	7.4	243
65	Molecular and Electronic Structures of Bis-(o-diiminobenzosemiquinonato)metal(II) Complexes (Ni,) Tj ETQq1 1 0.784314 rgBT /Overlock Journal of the American Chemical Society, 2003, 125, 9116-9128.	14.1	240
66	Calculating Absorption Shifts for Retinal Proteins:Â Computational Challenges. Journal of Physical Chemistry B, 2005, 109, 3606-3615.	2.6	240
67	Decomposition of Intermolecular Interaction Energies within the Local Pair Natural Orbital Coupled Cluster Framework. Journal of Chemical Theory and Computation, 2016, 12, 4778-4792.	5.4	240
68	MCDC-Term Signs, Saturation Behavior, and Determination of Band Polarizations in Randomly Oriented Systems with SpinSâ‰¥1/2. Applications toS=1/2andS=5/2. Inorganic Chemistry, 1999, 38, 1847-1865.	4.1	231
69	Calibration of Modern Density Functional Theory Methods for the Prediction of ⁵⁷Fe MÃ¶ssbauer Isomer Shifts: Meta-GGA and Double-Hybrid Functionals. Inorganic Chemistry, 2009, 48, 784-785.	4.1	230
70	Performance of Nonrelativistic and Quasi-Relativistic Hybrid DFT for the Prediction of Electric and Magnetic Hyperfine Parameters in 57Fe MÃ¶ssbauer Spectra. Inorganic Chemistry, 2005, 44, 2245-2254.	4.1	220
71	Sparse mapsâ€”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.	2.9	218
72	Molecular and Electronic Structure of Four- and Five-Coordinate Cobalt Complexes Containing Twoo-Phenylenediamine- or Twoo-Aminophenol-Type Ligands at Various Oxidation Levels: An Experimental, Density Functional, and Correlated ab initio Study. Chemistry - A European Journal, 2005, 11, 204-224.	3.8	216

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73	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.	2.9	216
74	Accurate Modeling of Spin-State Energetics in Spin-Crossover Systems with Modern Density Functional Theory. Inorganic Chemistry, 2010, 49, 772-774.	4.1	215
75	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, 3635-3648.	14.1	211
76	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, 2783-2797.	3.8	208
77	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, 3060-3073.	5.4	206
78	Covalency and chemical bonding in transition metal complexes: An ab initio based ligand field perspective. Coordination Chemistry Reviews, 2017, 344, 2-25.	19.2	203
79	Analysis of Reaction Channels for Alkane Hydroxylation by Nonheme Iron(IV)â€“Oxo Complexes. Angewandte Chemie - International Edition, 2010, 49, 5717-5720.	14.2	201
80	Time-dependent density functional calculations of ligand K-edge X-ray absorption spectra. Inorganica Chimica Acta, 2008, 361, 965-972.	2.5	200
81	Spectroscopic and Computational Evaluation of the Structure of the High-Spin Fe(IV)-Oxo Intermediates in Taurine: Î±-Ketoglutarate Dioxygenase fromEscherichia coliand Its His99Ala Ligand Variant. Journal of the American Chemical Society, 2007, 129, 6168-6179.	14.1	198
82	Structural, Spectroscopic, and Computational Study of an Octahedral, Non-Heme {Feâ”NO}6-8Series:Â [Fe(NO)(cyclam-ac)]2+/+/0. Journal of the American Chemical Society, 2004, 126, 5138-5153.	14.1	197
83	Calculating the Electron Paramagnetic Resonance Parameters of Exchange Coupled Transition Metal Complexes Using Broken Symmetry Density Functional Theory:Â Application to a MnIII/MnIVModel Compound. Journal of the American Chemical Society, 2004, 126, 2613-2622.	14.1	195
84	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.	2.6	193
85	Spinâ”Spin Contributions to the Zero-Field Splitting Tensor in Organic Triplets, Carbenes and BiradicalsA Density Functional and Ab Initio Study. Journal of Physical Chemistry A, 2006, 110, 12267-12275.	2.5	191
86	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.	2.5	190
87	Efficient time-dependent density functional theory approximations for hybrid density functionals: Analytical gradients and parallelization. Journal of Chemical Physics, 2011, 134, 054116.	2.9	187
88	The Electronic Structure of CuA:â€‰ A Novel Mixed-Valence Dinuclear Copper Electron-Transfer Center. Journal of the American Chemical Society, 1996, 118, 11501-11514.	14.1	180
89	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.	5.4	180
90	The Electronic Structure of the Isoelectronic, Square-Planar Complexes [FeII(L)2]2-and [CoIII(LBu)2]-(L2-and (LBu)2-= Benzene-1,2-dithiolates):Â An Experimental and Density Functional Theoretical Study. Journal of the American Chemical Society, 2005, 127, 4403-4415.	14.1	178

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91	Electronic structure analysis of multistate reactivity in transition metal catalyzed reactions: the case of Câ€“H bond activation by non-heme iron(iv)â€“oxo cores. Physical Chemistry Chemical Physics, 2013, 15, 8017.	2.8	178
92	Comparison of density functionals for energy and structural differences between the high- [5T2g:â€Š(t2g)4(eg)2] and low- [1A1g:â€Š(t2g)6(eg)0] spin states of the hexaquoferrous cation [Fe(H2O)6]2+. Journal of Chemical Physics, 2004, 120, 9473-9486.	2.9	177
93	Analytic derivatives for perturbatively corrected â€œdouble hybridâ€• density functionals: Theory, implementation, and applications. Journal of Chemical Physics, 2007, 126, 124115.	2.9	176
94	Accurate Theoretical Chemistry with Coupled Pair Models. Accounts of Chemical Research, 2009, 42, 641-648.	15.7	175
95	Xâ€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, 4989-4992.	14.2	170
96	Fully Automated Quantumâ€Chemistryâ€Based Computation of Spinâ€“Spinâ€Coupled Nuclear Magnetic Resonance Spectra. Angewandte Chemie - International Edition, 2017, 56, 14763-14769.	14.2	169
97	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.	2.9	168
98	A five-coordinate Mn(<scp>iv</scp>) intermediate in biological water oxidation: spectroscopic signature and a pivot mechanism for water binding. Chemical Science, 2016, 7, 72-84.	7.5	168
99	How to Build Molecules with Large Magnetic Anisotropy. Chemistry - A European Journal, 2009, 15, 4078-4087.	3.8	166
100	Identification of a spin-coupled Mo(<scp>iii</scp>) in the nitrogenase ironâ€“molybdenum cofactor. Chemical Science, 2014, 5, 3096-3103.	7.5	166
101	NAMD goes quantum: an integrative suite for hybrid simulations. Nature Methods, 2018, 15, 351-354.	19.2	166
102	The Purple Mixed-Valence CuACenter in Nitrous-oxide Reductase:Â 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.	14.1	165
103	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, 044110.	2.9	160
104	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, 18280-18285.	7.4	158
105	Detailed Spectroscopic and Theoretical Studies on [Fe(EDTA)(O2)]3-:Â Electronic Structure of the Side-on Ferricâ^'Peroxide Bond and Its Relevance to Reactivity. Journal of the American Chemical Society, 1998, 120, 12829-12848.	14.1	157
106	Quantum chemical calculations of spectroscopic properties of metalloproteins and model compounds: EPR and MÃ¶ssbauer properties. Current Opinion in Chemical Biology, 2003, 7, 125-135.	6.2	155
107	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.	5.4	155
108	Silicaâ€Protectionâ€Assisted Encapsulation of Cu₂O Nanocubes into a Metalâ€“Organic Framework (ZIFâ€8) To Provide a Composite Catalyst. Angewandte Chemie - International Edition, 2018, 57, 6834-6837.	14.2	153

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109	Detailed Ab Initio First-Principles Study of the Magnetic Anisotropy in a Family of Trigonal Pyramidal Iron(II) Pyrrolide Complexes. Inorganic Chemistry, 2011, 50, 7460-7477.	4.1	151
110	Ammonia binding to the oxygen-evolving complex of photosystem II identifies the solvent-exchangeable oxygen bridge (Ì¼-oxo) of the manganese tetramer. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 15561-15566.	7.4	150
111	Electronic Structure of Activated Bleomycin:â€‰ Oxygen Intermediates in Heme versus Non-Heme Iron. Journal of the American Chemical Society, 2000, 122, 11703-11724.	14.1	148
112	The Geometric and Electronic Structure of [(cyclam-acetato)Fe(N)]+: A Genuine Iron(V) Species with a Ground-State SpinS=1/2. Angewandte Chemie - International Edition, 2005, 44, 2908-2912.	14.2	146
113	The Mechanism of Homogeneous CO₂ Reduction by Ni(cyclam): Product Selectivity, Concerted Protonâ€“Electron Transfer and Câ€“O Bond Cleavage. Inorganic Chemistry, 2014, 53, 7500-7507.	4.1	145
114	On the theoretical prediction of fluorescence rates from first principles using the path integral approach. Journal of Chemical Physics, 2018, 148, 034104.	2.9	144
115	SparseMapsâ€”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.	2.9	142
116	Theoretical bioinorganic chemistry: the electronic structure makes a difference. Current Opinion in Chemical Biology, 2007, 11, 134-141.	6.2	141
117	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.	5.4	141
118	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 spinâ€“orbit coupled configuration interaction approaches. Physical Chemistry Chemical Physics, 2013, 15, 7260.	2.8	139
119	<scp>Allâ€electron</scp> scalar relativistic basis sets for the elements Rbâ€“Xe. Journal of Computational Chemistry, 2020, 41, 1842-1849.	3.4	138
120	Palladium-catalysed electrophilic aromatic Câ€“H fluorination. Nature, 2018, 554, 511-514.	35.3	137
121	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, 716-726.	3.6	135
122	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	133
123	SparseMapsâ€”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.	2.9	133
124	Square Planar vs Tetrahedral Coordination in Diamagnetic Complexes of Nickel(II) Containing Two Bidentate Ï€-Radical Monoanions. Inorganic Chemistry, 2005, 44, 3636-3656.	4.1	132
125	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, 10750-10758.	2.5	132
126	Revisiting the MÃ¶ssbauer Isomer Shifts of the FeMoco Cluster of Nitrogenase and the Cofactor Charge. Inorganic Chemistry, 2017, 56, 1470-1477.	4.1	132

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127	All-electron scalar relativistic basis sets for the 6p elements. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	128
128	KÎ² Mainline X-ray Emission Spectroscopy as an Experimental Probe of Metalâ€“Ligand Covalency. Journal of the American Chemical Society, 2014, 136, 9453-9463.	14.1	128
129	Theoretical Study of Ligand Superhyperfine Structure. Application to Cu(II) Complexes. Journal of Physical Chemistry A, 2001, 105, 4290-4299.	2.5	127
130	o-Iminobenzosemiquinonato(1â˙) and o-Amidophenolato(2â˙) Complexes of Palladium(II) and Platinum(II):â€‰ A Combined Experimental and Density Functional Theoretical Study. Inorganic Chemistry, 2002, 41, 4295-4303.	4.1	127
131	Improved Segmented All-Electron Relativistically Contracted Basis Sets for the Lanthanides. Journal of Chemical Theory and Computation, 2016, 12, 1148-1156.	5.4	125
132	A New Quantum Chemical Approach to the Magnetic Properties of Oligonuclear Transitionâ€Metal Complexes: Application to a Model for the Tetranuclear Manganese Cluster of Photosystemâ€…II. Chemistry - A European Journal, 2009, 15, 5108-5123.	3.8	124
133	Chemical applications carried out by local pair natural orbital based coupled-cluster methods. Chemical Society Reviews, 2014, 43, 5032-5041.	39.0	123
134	The Ligand Field of the Azido Ligand: Insights into Bonding Parameters and Magnetic Anisotropy in a Co(II)â€“Azido Complex. Journal of the American Chemical Society, 2015, 137, 1993-2005.	14.1	123
135	A Systematic Density Functional Study of the Zero-Field Splitting in Mn(II) Coordination Compounds. Inorganic Chemistry, 2008, 47, 134-142.	4.1	122
136	Structure of the oxygen-evolving complex of photosystem II: information on the S2 state through quantum chemical calculation of its magnetic properties. Physical Chemistry Chemical Physics, 2009, 11, 6788.	2.8	122
137	DFT exchange: sharing perspectives on the workhorse of quantum chemistry and materials science. Physical Chemistry Chemical Physics, 2022, 24, 28700-28781.	2.8	122
138	Electronic Structure and Reactivity of Low-Spin Fe(III)â˙Hydroperoxo Complexes:â€‰ Comparison to Activated Bleomycin. Journal of the American Chemical Society, 2002, 124, 10810-10822.	14.1	121
139	Hydrogen Bond Geometries from Electron Paramagnetic Resonance and Electronâ˙Nuclear Double Resonance Parameters:â€‰ Density Functional Study of Quinone Radical Anionâ˙Solvent Interactions. Journal of the American Chemical Society, 2004, 126, 3280-3290.	14.1	120
140	Manganese KÎ² X-ray Emission Spectroscopy As a Probe of Metalâ€“Ligand Interactions. Inorganic Chemistry, 2011, 50, 8397-8409.	4.1	120
141	Interaction of Radical Pairs Through-Bond and Through-Space: Scope and Limitations of the Pointâ˙Dipole Approximation in Electron Paramagnetic Resonance Spectroscopy. Journal of the American Chemical Society, 2009, 131, 10092-10106.	14.1	119
142	Assessment of n-Electron Valence State Perturbation Theory for Vertical Excitation Energies. Journal of Chemical Theory and Computation, 2013, 9, 3567-3580.	5.4	119
143	Quantum chemical studies of Câ€“H activation reactions by high-valent nonheme iron centers. Current Opinion in Chemical Biology, 2009, 13, 89-98.	6.2	118
144	Towards a pair natural orbital coupled cluster method for excited states. Journal of Chemical Physics, 2016, 145, 034102.	2.9	118

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