Martin Kaupp

List of Publications by Year
in descending order

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379	18,026	12330	26613
papers	citations	69 h-index	107 g-index

418	418	418	10970
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. Journal of Chemical Physics, 2020, 152, 184107.	3.0	616
2	Pseudopotential approaches to Ca, Sr, and Ba hydrides. Why are some alkaline earth MX2compounds bent?. Journal of Chemical Physics, 1991, 94, 1360-1366.	3.0	562
3	How Do Spin-Orbit-Induced Heavy-Atom Effects on NMR Chemical Shifts Function? Validation of a Simple Analogy to Spin-Spin Coupling by Density Functional Theory (DFT) Calculations on Some Iodo Compounds. Chemistry - A European Journal, 1998, 4, 118-126.	3.3	344
4	Exciton Trapping in Ï€-Conjugated Materials: A Quantum-Chemistry-Based Protocol Applied to Perylene Bisimide Dye Aggregates. Journal of the American Chemical Society, 2008, 130, 12858-12859.	13.7	290
5	The DFT route to NMR chemical shifts. Journal of Computational Chemistry, 1999, 20, 91-105.	3.3	274
6	A Critical Validation of Density Functional and Coupled-Cluster Approaches for the Calculation of EPR Hyperfine Coupling Constants in Transition Metal Complexes. Journal of Physical Chemistry A, 1999, 103, 9966-9983.	2.5	271
7	From Bis(silylene) and Bis(germylene) Pincer-Type Nickel(II) Complexes to Isolable Intermediates of the Nickel-Catalyzed Sonogashira Cross-Coupling Reaction. Journal of the American Chemical Society, 2013, 135, 15617-15626.	13.7	232
8	Density Functional Calculations of Electronicg-Tensors Using Spinâ^'Orbit Pseudopotentials and Mean-Field All-Electron Spinâ^'Orbit Operators. Journal of the American Chemical Society, 2000, 122, 9206-9218.	13.7	222
9	A fully relativistic method for calculation of nuclear magnetic shielding tensors with a restricted magnetically balanced basis in the framework of the matrix Diracâ€"Kohnâ€"Sham equation. Journal of Chemical Physics, 2008, 128, 104101.	3.0	196
10	A Reliable Quantum-Chemical Protocol for the Characterization of Organic Mixed-Valence Compounds. Journal of the American Chemical Society, 2009, 131, 16292-16302.	13.7	184
11	The highest oxidation states of the transition metal elements. Coordination Chemistry Reviews, 2009, 253, 606-624.	18.8	183
12	Calculation of electronic g-tensors for transition metal complexes using hybrid density functionals and atomic meanfield spin-orbit operators. Journal of Computational Chemistry, 2002, 23, 794-803.	3.3	182
13	The question of bending of the alkaline earth dihalides MX2 (M = beryllium, magnesium, calcium,) Tj ETQq1 1 0.784314 rgBT /Overloc of the American Chemical Society, 1991, 113, 6012-6020.	13.7	180
14	Quantum-chemical insights into mixed-valence systems: within and beyond the Robinâ€"Day scheme. Chemical Society Reviews, 2014, 43, 5067-5088.	38.1	168
15	Where Is the Spin? Understanding Electronic Structure andg-Tensors for Ruthenium Complexes with Redox-Active Quinonoid Ligands. Journal of the American Chemical Society, 2005, 127, 11399-11413.	13.7	164
16	â€œNonâ€VSEPRâ€•Structures and Bonding in d⁰Systems. Angewandte Chemie - International Edition, 2001, 40, 3534-3565.	13.8	158
17	Mechanisms of EPR Hyperfine Coupling in Transition Metal Complexes. Journal of the American Chemical Society, 2000, 122, 11900-11913.	13.7	148
18	From silicon(II)-based dioxygen activation to adducts of elusive dioxasiliranes and sila-ureas stable at room temperature. Nature Chemistry, 2010, 2, 577-580.	13.6	140

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19	Ab initio study of structures and stabilities of substituted lead compounds. Why is inorganic lead chemistry dominated by PbII but organolead chemistry by PbIV?. Journal of the American Chemical Society, 1993, 115, 1061-1073.	13.7	132
20	Carboalumination of a chromiumâ€“chromium quintuple bond. Nature Chemistry, 2009, 1, 322-325.	13.6	131
21	Mercury Is a Transition Metal: The First Experimental Evidence for HgF₄. Angewandte Chemie - International Edition, 2007, 46, 8371-8375.	13.8	126
22	13C NMR Study of Halogen Bonding of Haloarenes:Â Measurements of Solvent Effects and Theoretical Analysisâ€¡. Journal of the American Chemical Society, 2004, 126, 4412-4419.	13.7	121
23	Computational and spectroscopic studies of organic mixed-valence compounds: where is the charge?. Physical Chemistry Chemical Physics, 2011, 13, 16973.	2.8	121
24	Relativistic Four-Component DFT Calculations of ¹H NMR Chemical Shifts in Transition-Metal Hydride Complexes: Unusual High-Field Shifts Beyond the Buckinghamâ€“Stephens Model. Journal of Physical Chemistry A, 2011, 115, 5654-5659.	2.5	120
25	The role of radial nodes of atomic orbitals for chemical bonding and the periodic table. Journal of Computational Chemistry, 2007, 28, 320-325.	3.3	119
26	Theoretical and experimental study of diamagnetic and paramagnetic products from thermal and light-induced alkyl transfer between zinc or magnesium dialkyls and 1,4-diaza-1,3-butadiene substrates. Journal of the American Chemical Society, 1991, 113, 5606-5618.	13.7	118
27	Validation of local hybrid functionals for TDDFT calculations of electronic excitation energies. Journal of Chemical Physics, 2016, 144, 074106.	3.0	117
28	A thermochemically competitive local hybrid functional without gradient corrections. Journal of Chemical Physics, 2007, 126, 011103.	3.0	113
29	Relativistic Heavy-Neighbor-Atom Effects on NMR Shifts: Concepts and Trends Across the Periodic Table. Chemical Reviews, 2020, 120, 7065-7103.	47.7	113
30	Spinâ€“orbit corrections to NMR shielding constants from density functional theory. How important are the two-electron terms?. Chemical Physics Letters, 1998, 296, 93-104.	2.6	112
31	The structural variations of monomeric alkaline earth MX2 compounds (M = calcium, strontium,) Tj ETQq1 1 0.784314 rgBT /Overlock 1 Chemical Society, 1992, 114, 491-497.	13.7	108
32	A Neutral, Monomeric Germanium(I) Radical. Journal of the American Chemical Society, 2011, 133, 10074-10077.	13.7	108
33	The equilibrium structures of monomeric Group 2 and lanthanide(II) metallocenes MCp2 (M = calcium,) Tj ETQq1 1 0.784314 rgBT /Ov American Chemical Society, 1992, 114, 8202-8208.	13.7	107
34	Metalâ€“Metal Distances at the Limit: Crâ€“Cr 1.73 Ã… â€“ the Importance of the Ligand and its Fine Tuning. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2009, 635, 1149-1152.	1.2	107
35	Combining NMR spectroscopy and quantum chemistry as tools to quantify spin density distributions in molecular magnetic compounds. Coordination Chemistry Reviews, 2009, 253, 2376-2386.	18.8	106
36	Activation of Ammonia by a Siâ•Ö Double Bond and Formation of a Unique Pair of Sila-Hemiaminal and Silanoic Amide Tautomers. Journal of the American Chemical Society, 2010, 132, 6912-6913.	13.7	106

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37	Understanding Ground- and Excited-State Properties of Perylene Tetracarboxylic Acid Bisimide Crystals by Means of Quantum Chemical Computations. Journal of the American Chemical Society, 2009, 131, 15660-15668.	13.7	104
38	Study of relativistic effects on nuclear shieldings using density-functional theory and spinâ€“orbit pseudopotentials. Journal of Chemical Physics, 2001, 114, 61.	3.0	101
39	Impact of Molecular Flexibility on Binding Strength and Self-Sorting of Chiral Ï€-Surfaces. Journal of the American Chemical Society, 2011, 133, 9580-9591.	13.7	101
40	Breakdown of Bond Length-Bond Strength Correlation: A Case Study. Angewandte Chemie - International Edition, 2000, 39, 4607-4609.	13.8	100
41	Chemistry is about energy and its changes: A critique of bond-length/bond-strength correlations. Coordination Chemistry Reviews, 2017, 344, 355-362.	18.8	99
42	Density functional calculations of NMR shielding tensors for paramagnetic systems with arbitrary spin multiplicity: Validation on 3d metallocenes. Journal of Chemical Physics, 2007, 126, 024107.	3.0	98
43	Local hybrid exchange-correlation functionals based on the dimensionless density gradient. Chemical Physics Letters, 2007, 440, 160-168.	2.6	98
44	Interpretation of 13C NMR chemical shifts in halomethyl cations. On the importance of spin-orbit coupling and electron correlation. Chemical Physics Letters, 1997, 265, 55-59.	2.6	95
45	Local hybrid functionals: Theory, implementation, and performance of an emerging new tool in quantum chemistry and beyond. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1378.	14.6	95
46	Density Functional Calculations of Electronic g-Tensors for Semiquinone Radical Anions. The Role of Hydrogen Bonding and Substituent Effects. Journal of the American Chemical Society, 2002, 124, 2709-2722.	13.7	94
47	Insight into the Mechanism of Carbonyl Hydrosilylation Catalyzed by Brookhartâ€™s Cationic Iridium(III) Pincer Complex. Journal of the American Chemical Society, 2014, 136, 6912-6915.	13.7	93
48	Dominance of Linear 2-Coordination in Mercury Chemistry: Quasirelativistic and Nonrelativistic ab Initio Pseudopotential Study of (HgX2)2 (X = F, Cl, Br, I, H). Inorganic Chemistry, 1994, 33, 2555-2564.	4.0	92
49	Relationships in the rotational barriers of all Group 14 ethane congeners H3X-YH3 (X, Y = C, Si, Ge, Sn,) Tj ETQq1 1 0.784314 rgBT /Ov Chemical Society, 1992, 114, 6791-6797.	13.7	90
50	Calculation of ligand NMR chemical shifts in transition-metal complexes using ab initio effective-core potentials and density functional theory. Chemical Physics Letters, 1995, 235, 382-388.	2.6	90
51	ReSpect: Relativistic spectroscopy DFT program package. Journal of Chemical Physics, 2020, 152, 184101.	3.0	90
52	Relativistic spin-orbit effects on hyperfine coupling tensors by density-functional theory. Journal of Chemical Physics, 2004, 120, 2127-2139.	3.0	89
53	Local hybrid functionals: An assessment for thermochemical kinetics. Journal of Chemical Physics, 2007, 127, 194102.	3.0	87
54	Origin of the Unique Stability of Condensed-Phase Hg22+. An ab Initio Investigation of MI and MII Species (M = Zn, Cd, Hg). Inorganic Chemistry, 1994, 33, 4179-4185.	4.0	86

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55	Reversible [4Fe-3S] cluster morphing in an O2-tolerant [NiFe] hydrogenase. Nature Chemical Biology, 2014, 10, 378-385.	8.0	85
56	Importance of the correlation contribution for local hybrid functionals: Range separation and self-interaction corrections. Journal of Chemical Physics, 2012, 136, 014111.	3.0	83
57	Reliable Quantum Chemical Prediction of the Localized/Delocalized Character of Organic Mixed-Valence Radical Anions. From Continuum Solvent Models to Direct-COSMO-RS. Journal of Chemical Theory and Computation, 2012, 8, 4189-4203.	5.3	83
58	Scalar Relativistic Effects on 17O NMR Chemical Shifts in Transition-Metal Oxo Complexes. An ab Initio ECP/DFT Study. Journal of the American Chemical Society, 1995, 117, 1851-1852.	13.7	82
59	The calculation of 17O chemical shielding in transition metal oxo complexes. I. Comparison of DFT and ab initio approaches, and mechanisms of relativity-induced shielding. Journal of Chemical Physics, 1997, 106, 9201-9212.	3.0	81
60	Giant Spinâ€Orbit Effects on NMR Shifts in Diamagnetic Actinide Complexes: Guiding the Search of Uranium(VI) Hydride Complexes in the Correct Spectral Range. Angewandte Chemie - International Edition, 2012, 51, 10884-10888.	13.8	81
61	Oxidation State +IV in Group 12 Chemistry. Ab Initio Study of Zinc(IV), Cadmium(IV), and Mercury(IV) Fluorides. Inorganic Chemistry, 1994, 33, 2122-2131.	4.0	80
62	The Structure of XeF6and of Compounds Isoelectronic with It. A Challenge to Computational Chemistry and to the Qualitative Theory of the Chemical Bond. Journal of the American Chemical Society, 1996, 118, 11939-11950.	13.7	79
63	The Structure of Hexamethyltungsten, W(CH3)6:â€‰ Distorted Trigonal Prismatic with C3 Symmetry. Journal of the American Chemical Society, 1996, 118, 3018-3024.	13.7	78
64	Mixedâ€Valence Ruthenium Complexes Rotating through a Conformational Robinâ€“Day Continuum. Chemistry - A European Journal, 2014, 20, 6895-6908.	3.3	76
65	Mechanism of the cooperative Siâ€“H bond activation at Ruâ€“S bonds. Chemical Science, 2015, 6, 4324-4334.	7.4	76
66	Density Functional Calculations of ⁵⁵Mn, ¹⁴N and ¹³C Electron Paramagnetic Resonance Parameters Support an Energetically Feasible Model System for the S₂ State of the Oxygenâ€Evolving Complex of Photosystem II. Chemistry - A European Journal, 2010, 16, 10424-10438.	3.3	73
67	Structure of the Oxygen-Rich Cluster Cation Al₂O₇⁺and its Reactivity toward Methane and Water. Journal of the American Chemical Society, 2011, 133, 16930-16937.	13.7	73
68	Density functional analysis of 13C and 1H chemical shifts and bonding in mercurimethanes and organomercury hydrides: The role of scalar relativistic, spin-orbit, and substituent effects. Journal of Chemical Physics, 1998, 108, 3648-3659.	3.0	72
69	Relativistic two-component calculations of electronic g-tensors that include spin polarization. Journal of Chemical Physics, 2005, 123, 244103.	3.0	72
70	The Family of Ferroceneâ€Stabilized Silylium Ions: Synthesis,29Siâ€…NMR Characterization, Lewis Acidity, Substituent Scrambling, and Quantumâ€Chemical Analyses. Chemistry - A European Journal, 2013, 19, 16579-16594.	3.3	69
71	Efficient Self-Consistent Implementation of Local Hybrid Functionals. Journal of Chemical Theory and Computation, 2015, 11, 1540-1548.	5.3	69
72	Towards improved local hybrid functionals by calibration of exchange-energy densities. Journal of Chemical Physics, 2014, 141, 204101.	3.0	68

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73	A Density Functional Study of EPR Parameters for Vanadyl Complexes Containing Schiff Base Ligands. Journal of Physical Chemistry B, 2001, 105, 12644-12652.	2.6	67
74	Validation study of meta-GGA functionals and of a model exchangeâ€“correlation potential in density functional calculations of EPR parameters. Physical Chemistry Chemical Physics, 2002, 4, 5467-5474.	2.8	67
75	A Rare Uranyl(VI)â€“Alkyl Ate Complex [Li(DME)_{1.5}]₂[UO₂(CH₂SiMe₃)₄] and Its Comparison with a Homoleptic Uranium(VI)â€“Hexaalkyl. Angewandte Chemie - International Edition, 2013, 52, 3259-3263.	13.8	67
76	[Pb5{Mo(CO)3}2]4â^': A Complex Containing a Planar Pb5Unit. Angewandte Chemie - International Edition, 2005, 44, 2092-2096.	13.8	66
77	Calculation of zero-field splitting parameters: Comparison of a two-component noncolinear spin-density-functional method and a one-component perturbational approach. Journal of Chemical Physics, 2006, 125, 054110.	3.0	66
78	Combined Spectroscopic and Quantum Chemical Study of [trans-Ru(Câ‰¡CC₆H₄R¹-4)₂(dppe)₂]ⁿ⁺ and [trans-Ru(Câ‰¡CC₆H₄R¹-4)(Câ‰¡CC₆H₄R²-4)(n = 0, 1) Complexes: Interpretations beyond the Lowest Energy Conformer Paradigm. Organometallics, 2014, 33, 4947-4963.	2.3	66
79	Systematic Experimental and Quantum Chemical Investigation into the Structures, the Stability, and the Spectroscopic Properties of Alkylindium(I) Compounds:â€‰ Tetrameric In4[C(SiMeRRâ€˜)3]4 versus Monomeric InC(SiMeRRâ€˜)3 Derivatives. Organometallics, 1998, 17, 5009-5017.	2.3	64
80	From local hybrid functionals to â€œlocalized local hybridâ€•potentials: Formalism and thermochemical tests. Journal of Chemical Physics, 2006, 124, 204102.	3.0	64
81	Formation and Characterization of the Iridium Tetroxide Molecule with Iridium in the Oxidation State +VIII. Angewandte Chemie - International Edition, 2009, 48, 7879-7883.	13.8	64
82	Squaraine Dyes as Efficient Coupling Bridges between Triarylamine Redox Centres. Chemistry - A European Journal, 2011, 17, 14147-14163.	3.3	64
83	Synthesis and Bonding in Carbene Complexes of an Unsymmetrical Dilithio Methandiide: A Combined Experimental and Theoretical Study. Chemistry - A European Journal, 2013, 19, 16729-16739.	3.3	64
84	Gaseous Mercury(IV) Fluoride, HgF4: An Ab Initio Study. Angewandte Chemie International Edition in English, 1993, 32, 861-863.	4.4	63
85	Density Functional Study of EPR Parameters and Spin-Density Distribution of Azurin and Other Blue Copper Proteins. Journal of Physical Chemistry B, 2007, 111, 8290-8304.	2.6	63
86	Spinâ^'Orbit Effects on Hyperfine Coupling Tensors in Transition Metal Complexes Using Hybrid Density Functionals and Accurate Spinâ^'Orbit Operators. Journal of Physical Chemistry A, 2004, 108, 5026-5033.	2.5	62
87	Refining the Interpretation of Nearâ€Infrared Band Shapes in a Polyynediyl Molecular Wire. Chemistry - A European Journal, 2013, 19, 9780-9784.	3.3	61
88	Multifrequency EPR Study and Density Functional g-Tensor Calculations of Persistent Organorhenium Radical Complexes. Journal of the American Chemical Society, 2002, 124, 10563-10571.	13.7	60
89	Ro-Vibrational Corrections to NMR Parameters. , 2004, , 153-173.		60
90	A Relativistic Quantum-Chemical Analysis of the trans Influence on ¹H NMR Hydride Shifts in Square-Planar Platinum(II) Complexes. Inorganic Chemistry, 2015, 54, 7199-7208.	4.0	60

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91	Ab Initio Molecular Dynamics Simulations and g-Tensor Calculations of Aqueous Benzosemiquinone Radical Anion:Â Effects of Regular and â€œT-Stackedâ€•Hydrogen Bonds. Journal of the American Chemical Society, 2004, 126, 9854-9861.	13.7	59
92	Do low-coordinated Group 1-3 cations Mn+Lm (Mn+ = potassium, rubidium cesium, calcium, strontium,) Tj ETQq0 0 0 rgBT /Overlock 10 noble-gas electron configuration favor regular or abnormal shapes?. The Journal of Physical Chemistry, 1992, 96, 7316-7323.	2.9	57
93	Understanding Substituent Effects on29Si Chemical Shifts and Bonding in Disilenes. A Quantum Chemical Analysisâ€. Organometallics, 2003, 22, 2442-2449.	2.3	57
94	Scalar relativistic calculations of hyperfine coupling tensors using the Douglasâ€“Krollâ€“Hess method. Chemical Physics Letters, 2004, 396, 268-276.	2.6	57
95	Development of a TDDFT-Based Protocol with Local Hybrid Functionals for the Screening of Potential Singlet Fission Chromophores. Journal of Chemical Theory and Computation, 2017, 13, 4984-4996.	5.3	57
96	Has AuF7Been Made?. Inorganic Chemistry, 2006, 45, 1228-1234.	4.0	56
97	Formal Oxidation State versus Partial Chargeâ€”A Comment. Angewandte Chemie International Edition in English, 1995, 34, 986-986.	4.4	55
98	The self-consistent implementation of exchange-correlation functionals depending on the local kinetic energy density. Chemical Physics Letters, 2003, 381, 495-504.	2.6	55
99	Validation of density functional methods for computing structures and energies of mercury(iv) complexesElectronic supplementary information (ESI) available: Structure of transition state for HgH4 dissociation and tables with CP-connections and transition state structures. See http://www.rsc.org/suppdata/cp/b3/b315019d/. Physical Chemistry Chemical Physics, 2004, 6, 1122.	2.8	55
100	Structure of the Nucleotide Radical Formed during Reaction of CDP/TTP with the E441Q-Î±2Î²2 ofE. coliRibonucleotide Reductase. Journal of the American Chemical Society, 2009, 131, 200-211.	13.7	55
101	The Nonoctahedral Structures of d0, d1, and d2 Hexamethyl Complexes. Chemistry - A European Journal, 1998, 4, 1678-1686.	3.3	54
102	The Function of Photosystem I. Quantum Chemical Insight into the Role of Tryptophanâ^'Quinone Interactions. Biochemistry, 2002, 41, 2895-2900.	2.5	54
103	Perturbational and ECP Calculation of Relativistic Effects in NMR Shielding and Spin-Spin Coupling. , 2004, , 209-226.		54
104	Relativistic Effects on NMR Chemical Shifts. Theoretical and Computational Chemistry, 2004, 14, 552-597.	0.4	54
105	Jacobsenâ€™s Catalyst for Hydrolytic Kinetic Resolution: Structure Elucidation of Paramagnetic Co(III) Salen Complexes in Solution via Combined NMR and Quantum Chemical Studies. Journal of the American Chemical Society, 2009, 131, 4172-4173.	13.7	54
106	Efficient Semi-numerical Implementation of Global and Local Hybrid Functionals for Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2015, 11, 4226-4237.	5.3	54
107	A Local Hybrid Functional with Wide Applicability and Good Balance between (De)Localization and Leftâ€“Right Correlation. Journal of Chemical Theory and Computation, 2020, 16, 5645-5657.	5.3	54
108	A Trimetallic Gold Boride Complex with a Fluxional Goldâ€“Boron Bond. Angewandte Chemie - International Edition, 2009, 48, 9735-9738.	13.8	53

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109	Ab Initio ECP/DFT Calculation and Interpretation of Carbon and Oxygen NMR Chemical Shift Tensors in Transitionâ€Metal Carbonyl Complexes. Chemistry - A European Journal, 1996, 2, 24-30.	3.3	52
110	First-Principles Calculations of Paramagnetic NMR Shifts. , 2004, , 325-338.		52
111	Scalar relativistic calculations of hyperfine coupling tensors using the Douglasâ€“Krollâ€“Hess method with a finite-size nucleus model. Physical Chemistry Chemical Physics, 2006, 8, 4079-4085.	2.8	52
112	Synthesis, Reactivity, and Electronic Structure of [n]Vanadoarenophanes: An Experimental and Theoretical Study. Journal of the American Chemical Society, 2008, 130, 11376-11393.	13.7	52
113	The Cluster Anion Si94â˜. Angewandte Chemie - International Edition, 1998, 37, 2359-2361.	13.8	51
114	Pseudoâ€Contact NMR Shifts over the Paramagnetic Metalloprotein CoMMPâ€12 from First Principles. Angewandte Chemie - International Edition, 2016, 55, 14713-14717.	13.8	51
115	Predicting the Localized/Delocalized Character of Mixed-Valence Diquinone Radical Anions. Toward the Right Answer for the Right Reason. Journal of Physical Chemistry A, 2012, 116, 10629-10637.	2.5	50
116	Structure of the Nitrogen-Centered Radical Formed during Inactivation ofE. coliRibonucleotide Reductase by 2â€˜-Azido-2â€˜-deoxyuridine-5â€˜-diphosphate:Â Trapping of the 3â€˜-Ketonucleotide. Journal of the American Chemical Society, 2005, 127, 7729-7738.	13.7	49
117	Understanding Structure and Bonding in Early Actinide 6d05f0MX6q(M = Thâ˜Np; X = H, F) Complexes in Comparison with Their Transition Metal 5d0Analogues. Journal of the American Chemical Society, 2005, 127, 2591-2599.	13.7	49
118	Diphosphines with Strongly Polarized Pâ˜P Bonds: Hybrids between Covalent Molecules and Donorâ˜Acceptor Adducts with Flexible Molecular Structures. Journal of the American Chemical Society, 2009, 131, 10763-10774.	13.7	49
119	Four-Component Relativistic Density Functional Theory Calculations of EPRg- and Hyperfine-Coupling Tensors Using Hybrid Functionals: Validation on Transition-Metal Complexes with Large Tensor Anisotropies and Higher-Order Spinâ€Orbit Effects. Journal of Physical Chemistry A, 2015, 119, 12892-12905.	2.5	49
120	Solid-State Nuclear Magnetic Resonance Spectroscopic and Quantum Chemical Investigation of13C and17O Chemical Shift Tensors,17O Nuclear Quadrupole Coupling Tensors, and Bonding in Transition-Metal Carbonyl Complexes and Clusters. Journal of the American Chemical Society, 1998, 120, 4771-4783.	13.7	48
121	The PI4+ cation has an extremely large negative 31P nuclear magnetic resonance chemical shift, due to spinâ€orbit coupling: A quantum-chemical prediction and its confirmation by solid-state nuclear magnetic resonance spectroscopy. Journal of Chemical Physics, 1999, 110, 3897-3902.	3.0	46
122	Phosphorus Chemical Shifts in a Nucleic Acid Backbone from Combined Molecular Dynamics and Density Functional Calculations. Journal of the American Chemical Society, 2010, 132, 17139-17148.	13.7	45
123	From Silylone to an Isolable Monomeric Silicon Disulfide Complex. Angewandte Chemie - International Edition, 2015, 54, 10254-10257.	13.8	45
124	New Zwitterionic Spirocyclic Î»5Si-Silicates with anSiX4C Skeleton (X = S, O) Containing Two Ligands of the Dithiolato(2â˜) or Diolato(2â˜) Type:Â Synthesis, Structure, and Bonding SituationÂ§. Organometallics, 2003, 22, 4104-4110.	2.3	44
125	Reaction of Pentadienyl Complexes with Metal Carbonyls:â€‰ Synthetic, Structural, and Theoretical Studies of Metallabenzene Ï€-Complexes. Organometallics, 2003, 22, 264-274.	2.3	44
126	Solvent effects on g-tensors of semiquinone radical anions: polarizable continuum versus cluster models. Theoretical Chemistry Accounts, 2004, 111, 132-140.	1.4	44

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127	What can we learn from the adiabatic connection formalism about local hybrid functionals?. Journal of Chemical Physics, 2008, 128, 214107.	3.0	44
128	An Isolable Silicon Dicarbonate Complex from Carbon Dioxide Activation with a Silylone. Angewandte Chemie - International Edition, 2017, 56, 1894-1897.	13.8	44
129	Iron versus Ruthenium: Clarifying the Electronic Differences between Prototypical Mixed-Valence Organometallic Butadiyndiyl Bridged Molecular Wires. Organometallics, 2018, 37, 1432-1445.	2.3	44
130	Local Hybrid Functionals with an Explicit Dependence on Spin Polarization. Journal of Physical Chemistry A, 2009, 113, 11898-11906.	2.5	43
131	A Combined Computational and Spectroelectrochemical Study of Platinum-Bridged Bis-Triarylamine Systems. Inorganic Chemistry, 2014, 53, 1544-1554.	4.0	43
132	New approaches for the calibration of exchange-energy densities in local hybrid functionals. Physical Chemistry Chemical Physics, 2016, 18, 21133-21144.	2.8	43
133	Wavelength selective polymer network formation of end-functional star polymers. Chemical Communications, 2016, 52, 1975-1978.	4.1	43
134	In Situ Study on the Wet Chemical Synthesis of Nanoscopic Pt Colloids by â€œReductive Stabilizationâ€â€. Journal of Physical Chemistry B, 2003, 107, 7507-7515.	2.6	42
135	Construction of local hybrid exchange-correlation potentials and their evaluation for nuclear shielding constants. Chemical Physics Letters, 2004, 386, 8-16.	2.6	42
136	Advances in local hybrid exchangeâ€“correlation functionals: from thermochemistry to magneticâ€“resonance parameters and hyperpolarizabilities. International Journal of Quantum Chemistry, 2011, 111, 2625-2638.	2.0	42
137	Giant spinâ€“orbit effects on ¹H and ¹³C NMR shifts for uranium(<scp>vi</scp>) complexes revisited: role of the exchangeâ€“correlation response kernel, bonding analyses, and new predictions. Physical Chemistry Chemical Physics, 2016, 18, 30462-30474.	2.8	42
138	Insights into transâ€Ligand and Spinâ€Orbit Effects on Electronic Structure and Ligand NMR Shifts in Transitionâ€Metal Complexes. Chemistry - A European Journal, 2017, 23, 9790-9803.	3.3	42
139	Experimental and theoretical studies of alkaline-earth metal coordination: x-ray crystal structures of calcium, strontium, and barium carbazoles and ab initio model calculations. Journal of the American Chemical Society, 1992, 114, 10880-10889.	13.7	41
140	Sn6(PR)6],[Sn3(Pr)2, and[Cu24(PR)12](R= Triorganoisilyl): New Tin and Copper Phosphanediyl Clusters. Angewandte Chemie International Edition in English, 1997, 36, 1894-1896.	4.4	41
141	On the Relation between Ï€ Bonding, Electronegativity, and Bond Angles in High-Valent Transition Metal Complexes. Chemistry - A European Journal, 1999, 5, 3631-3643.	3.3	41
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