Martin Kaupp

List of Publications by Citations

385 papers	15,051 citations	64 h-index	97 g-index
416 ext. papers	16,569 ext. citations	7.1 avg, IF	6.8 L-index

#	Paper	IF	Citations
385	Pseudopotential approaches to Ca, Sr, and Ba hydrides. Why are some alkaline earth MX2 compounds bent?. *Journal of Chemical Physics*, **1991**, 94, 1360-1366	3.9	502
384	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	4.8	305
383	Exciton trapping in pi-conjugated materials: a quantum-chemistry-based protocol applied to perylene bisimide dye aggregates. *Journal of the American Chemical Society*, **2008**, 130, 12858-9	16.4	258
382	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. *Journal of Chemical Physics*, **2020**, 152, 184107	3.9	255
381	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	2.8	251
380	The DFT route to NMR chemical shifts. *Journal of Computational Chemistry*, **1999**, 20, 91-105	3.5	245
379	Density Functional Calculations of Electronic g-Tensors Using Spin□Orbit Pseudopotentials and Mean-Field All-Electron Spin□Orbit Operators. *Journal of the American Chemical Society*, **2000**, 122, 9206-9218	16.4	211
378	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, 15617-26	16.4	189
377	A fully relativistic method for calculation of nuclear magnetic shielding tensors with a restricted magnetically balanced basis in the framework of the matrix Dirac-Kohn-Sham equation. *Journal of Chemical Physics*, **2008**, 128, 104101	3.9	169
376	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	3.5	166
375	The question of bending of the alkaline earth dihalides MX2 (M = beryllium, magnesium, calcium, strontium, barium; X = fluorine, chlorine, bromine, iodine). An ab initio pseudopotential study. *Journal of the American Chemical Society*, **1991**, 113, 6012-6020	16.4	159
374	A reliable quantum-chemical protocol for the characterization of organic mixed-valence compounds. *Journal of the American Chemical Society*, **2009**, 131, 16292-302	16.4	154
373	Where is the spin? Understanding electronic structure and g-tensors for ruthenium complexes with redox-active quinonoid ligands. *Journal of the American Chemical Society*, **2005**, 127, 11399-413	16.4	148
372	The highest oxidation states of the transition metal elements. *Coordination Chemistry Reviews*, **2009**, 253, 606-624	23.2	145
371	Quantum-chemical insights into mixed-valence systems: within and beyond the Robin-Day scheme. *Chemical Society Reviews*, **2014**, 43, 5067-88	58.5	132
370	Mechanisms of EPR Hyperfine Coupling in Transition Metal Complexes. *Journal of the American Chemical Society*, **2000**, 122, 11900-11913	16.4	132
369	"Non-VSEPR" Structures and Bonding in d(0) Systems. *Angewandte Chemie - International Edition*, **2001**, 40, 3534-3565	16.4	131

368	From silicon(II)-based dioxygen activation to adducts of elusive dioxasiliranes and sila-ureas stable at room temperature. *Nature Chemistry*, **2010**, 2, 577-80	17.6	128
367	Carboalumination of a chromium□chromium quintuple bond. *Nature Chemistry*, **2009**, 1, 322-5	17.6	119
366	13C NMR study of halogen bonding of haloarenes: measurements of solvent effects and theoretical analysis. *Journal of the American Chemical Society*, **2004**, 126, 4412-9	16.4	115
365	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	16.4	111
364	Relativistic four-component DFT calculations of 1H NMR chemical shifts in transition-metal hydride complexes: unusual high-field shifts beyond the Buckingham-Stephens model. *Journal of Physical Chemistry A*, **2011**, 115, 5654-9	2.8	106
363	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	16.4	106
362	Mercury is a transition metal: the first experimental evidence for HgF(4). *Angewandte Chemie - International Edition*, **2007**, 46, 8371-5	16.4	103
361	Computational and spectroscopic studies of organic mixed-valence compounds: where is the charge?. *Physical Chemistry Chemical Physics*, **2011**, 13, 16973-86	3.6	102
360	Activation of ammonia by a Si=O double bond and formation of a unique pair of sila-hemiaminal and silanoic amide tautomers. *Journal of the American Chemical Society*, **2010**, 132, 6912-3	16.4	102
359	Spin□orbit corrections to NMR shielding constants from density functional theory. How important are the two-electron terms?. *Chemical Physics Letters*, **1998**, 296, 93-104	2.5	102
358	A thermochemically competitive local hybrid functional without gradient corrections. *Journal of Chemical Physics*, **2007**, 126, 011103	3.9	101
357	Metal□Metal Distances at the Limit: Cr□Cr 1.73 □□the Importance of the Ligand and its Fine Tuning. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2009**, 635, 1149-1152	1.3	98
356	The structural variations of monomeric alkaline earth MX2 compounds (M = calcium, strontium, barium; X = Li, BeH, BH2, CH3, NH2, OH, F). An ab initio pseudopotential study. *Journal of the American Chemical Society*, **1992**, 114, 491-497	16.4	97
355	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, 15660-8	16.4	94
354	Combining NMR spectroscopy and quantum chemistry as tools to quantify spin density distributions in molecular magnetic compounds. *Coordination Chemistry Reviews*, **2009**, 253, 2376-2386	23.2	93
353	Validation of local hybrid functionals for TDDFT calculations of electronic excitation energies. *Journal of Chemical Physics*, **2016**, 144, 074106	3.9	93
352	Breakdown of Bond Length-Bond Strength Correlation: A Case Study. *Angewandte Chemie - International Edition*, **2000**, 39, 4607-4609	16.4	92
351	The equilibrium structures of monomeric Group 2 and lanthanide(II) metallocenes MCp2 (M = calcium, strontium, barium, samarium, europium, ytterbium) studied by ab initio calculations. *Journal of the American Chemical Society*, **1992**, 114, 8202-8208	16.4	91

350	Local hybrid exchange-correlation functionals based on the dimensionless density gradient. *Chemical Physics Letters*, **2007**, 440, 160-168	2.5	90
349	Study of relativistic effects on nuclear shieldings using density-functional theory and spin□orbit pseudopotentials. *Journal of Chemical Physics*, **2001**, 114, 61	3.9	90
348	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, 2709-22	16.4	89
347	Impact of molecular flexibility on binding strength and self-sorting of chiral □urfaces. *Journal of the American Chemical Society*, **2011**, 133, 9580-91	16.4	87
346	A neutral, monomeric germanium(I) radical. *Journal of the American Chemical Society*, **2011**, 133, 10074-7	16.4	86
345	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	3.9	85
344	The role of radial nodes of atomic orbitals for chemical bonding and the periodic table. *Journal of Computational Chemistry*, **2007**, 28, 320-5	3.5	84
343	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	2.5	83
342	Relativistic spin-orbit effects on hyperfine coupling tensors by density-functional theory. *Journal of Chemical Physics*, **2004**, 120, 2127-39	3.9	83
341	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	5.1	82
340	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	5.1	82
339	Insight into the mechanism of carbonyl hydrosilylation catalyzed by Brookhart's cationic iridium(III) pincer complex. *Journal of the American Chemical Society*, **2014**, 136, 6912-5	16.4	81
338	Relationships in the rotational barriers of all Group 14 ethane congeners H3X-YH3 (X, Y = C, Si, Ge, Sn, Pb). Comparisons of ab initio pseudopotential and all-electron results. *Journal of the American Chemical Society*, **1992**, 114, 6791-6797	16.4	80
337	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	2.5	79
336	Local hybrid functionals: an assessment for thermochemical kinetics. *Journal of Chemical Physics*, **2007**, 127, 194102	3.9	75
335	Giant spin-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, 10884-8	16.4	73
334	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	16.4	72
333	The Structure of Hexamethyltungsten, W(CH3)6: Distorted Trigonal Prismatic with C3 Symmetry. *Journal of the American Chemical Society*, **1996**, 118, 3018-3024	16.4	72

332	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	5.1	72
331	Reversible [4Fe-3S] cluster morphing in an O(2)-tolerant [NiFe] hydrogenase. *Nature Chemical Biology*, **2014**, 10, 378-85	11.7	70
330	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, 4189-203	6.4	70
329	Mechanism of the cooperative Si-H bond activation at Ru-S bonds. *Chemical Science*, **2015**, 6, 4324-4334	9.4	69
328	Structure of the oxygen-rich cluster cation Al2O7+ and its reactivity toward methane and water. *Journal of the American Chemical Society*, **2011**, 133, 16930-7	16.4	69
327	Density functional calculations of (55)Mn, (14)N and (13)C electron paramagnetic resonance parameters support an energetically feasible model system for the S(2) state of the oxygen-evolving complex of photosystem II. *Chemistry - A European Journal*, **2010**, 16, 10424-38	4.8	68
326	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	3.9	68
325	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	3.9	68
324	The family of ferrocene-stabilized silylium ions: synthesis, 29Si NMR characterization, Lewis acidity, substituent scrambling, and quantum-chemical analyses. *Chemistry - A European Journal*, **2013**, 19, 16579-94	4.8	67
323	Relativistic two-component calculations of electronic g-tensors that include spin polarization. *Journal of Chemical Physics*, **2005**, 123, 244103	3.9	65
322	A Density Functional Study of EPR Parameters for Vanadyl Complexes Containing Schiff Base Ligands. *Journal of Physical Chemistry B*, **2001**, 105, 12644-12652	3.4	64
321	From local hybrid functionals to "localized local hybrid" potentials: formalism and thermochemical tests. *Journal of Chemical Physics*, **2006**, 124, 204102	3.9	63
320	Validation study of meta-GGA functionals and of a model exchange□correlation potential in density functional calculations of EPR parameters. *Physical Chemistry Chemical Physics*, **2002**, 4, 5467-5474	3.6	63
319	Synthesis and bonding in carbene complexes of an unsymmetrical dilithio methandiide: a combined experimental and theoretical study. *Chemistry - A European Journal*, **2013**, 19, 16729-39	4.8	62
318	Importance of the correlation contribution for local hybrid functionals: range separation and self-interaction corrections. *Journal of Chemical Physics*, **2012**, 136, 014111	3.9	62
317	The Structure of XeF6 and 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	16.4	62
316	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	7.9	60
315	Squaraine dyes as efficient coupling bridges between triarylamine redox centres. *Chemistry - A European Journal*, **2011**, 17, 14147-63	4.8	60

314	[Pb5{Mo(CO)3}2]4-: a complex containing a planar Pb5 unit. *Angewandte Chemie - International Edition*, **2005**, 44, 2092-6	16.4	60
313	Mixed-valence ruthenium complexes rotating through a conformational Robin-Day continuum. *Chemistry - A European Journal*, **2014**, 20, 6895-908	4.8	59
312	A rare uranyl(VI)-alkyl ate complex [Li(DME)1.5]2[UO2(CH2SiMe3)4] and its comparison with a homoleptic uranium(VI)-hexaalkyl. *Angewandte Chemie - International Edition*, **2013**, 52, 3259-63	16.4	59
311	Density functional study of EPR parameters and spin-density distribution of azurin and other blue copper proteins. *Journal of Physical Chemistry B*, **2007**, 111, 8290-304	3.4	59
310	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	3.9	59
309	Spin□Orbit Effects on Hyperfine Coupling Tensors in Transition Metal Complexes Using Hybrid Density Functionals and Accurate Spin□Orbit Operators. *Journal of Physical Chemistry A*, **2004**, 108, 5026-5033	2.8	59
308	Gaseous Mercury(IV) Fluoride, HgF4: An Ab Initio Study. *Angewandte Chemie International Edition in English*, **1993**, 32, 861-863		59
307	Chemistry is about energy and its changes: A critique of bond-length/bond-strength correlations. *Coordination Chemistry Reviews*, **2017**, 344, 355-362	23.2	58
306	Combined Spectroscopic and Quantum Chemical Study of [trans-Ru(C?CC6H4R1-4)2(dppe)2]n+ and [trans-Ru(C?CC6H4R1-4)(C?CC6H4R2-4)(dppe)2]n+ (n = 0, 1) Complexes: Interpretations beyond the Lowest Energy Conformer Paradigm. *Organometallics*, **2014**, 33, 4947-4963	3.8	58
305	Formation and characterization of the iridium tetroxide molecule with iridium in the oxidation state +VIII. *Angewandte Chemie - International Edition*, **2009**, 48, 7879-83	16.4	56
304	Do low-coordinated Group 1-3 cations Mn+Lm (Mn+ = potassium, rubidium cesium, calcium, strontium, barium, scandium, yttrium, lanthanum; L = ammonia, water, hydrogen fluoride; m = 1-3) with a formal noble-gas electron configuration favor regular or abnormal shapes?. *The Journal of Physical Chemistry*, **1992**, 96, 7316-7323		56
303	Understanding Substituent Effects on 29Si Chemical Shifts and Bonding in Disilenes. A Quantum Chemical Analysis□ *Organometallics*, **2003**, 22, 2442-2449	3.8	55
302	Multifrequency EPR study and density functional g-tensor calculations of persistent organorhenium radical complexes. *Journal of the American Chemical Society*, **2002**, 124, 10563-71	16.4	55
301	A Relativistic Quantum-Chemical Analysis of the trans Influence on (1)H NMR Hydride Shifts in Square-Planar Platinum(II) Complexes. *Inorganic Chemistry*, **2015**, 54, 7199-208	5.1	54
300	Systematic Experimental and Quantum Chemical Investigation into the Structures, the Stability, and the Spectroscopic Properties of Alkylindium(I) Compounds: Tetrameric In4[C(SiMeRR□3]4 versus Monomeric InC(SiMeRR□3 Derivatives□ *Organometallics*, **1998**, 17, 5009-5017	3.8	54
299	Ro-Vibrational Corrections to NMR Parameters **2004**, 153-173		53
298	Validation of density functional methods for computing structures and energies of mercury(IV) complexes. *Physical Chemistry Chemical Physics*, **2004**, 6, 1122	3.6	53
297	Ab initio molecular dynamics simulations and g-tensor calculations of aqueous benzosemiquinone radical anion: effects of regular and "T-stacked" hydrogen bonds. *Journal of the American Chemical Society*, **2004**, 126, 9854-61	16.4	53

296	Scalar relativistic calculations of hyperfine coupling tensors using the Douglas-Kroll-Hess method. *Chemical Physics Letters*, **2004**, 396, 268-276	2.5	52
295	Refining the interpretation of near-infrared band shapes in a polyynediyl molecular wire. *Chemistry - A European Journal*, **2013**, 19, 9780-4	4.8	51
294	A trimetallic gold boride complex with a fluxional gold-boron bond. *Angewandte Chemie - International Edition*, **2009**, 48, 9735-8	16.4	51
293	Synthesis, reactivity, and electronic structure of [n]vanadoarenophanes: an experimental and theoretical study. *Journal of the American Chemical Society*, **2008**, 130, 11376-93	16.4	51
292	Has AuF7 been made?. *Inorganic Chemistry*, **2006**, 45, 1228-34	5.1	51
291	The self-consistent implementation of exchange-correlation functionals depending on the local kinetic energy density. *Chemical Physics Letters*, **2003**, 381, 495-504	2.5	51
290	The function of photosystem I. Quantum chemical insight into the role of tryptophan-quinone interactions. *Biochemistry*, **2002**, 41, 2895-900	3.2	51
289	Jacobsen'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, 4172-3	16.4	50
288	Structure of the nucleotide radical formed during reaction of CDP/TTP with the E441Q-alpha2beta2 of E. coli ribonucleotide reductase. *Journal of the American Chemical Society*, **2009**, 131, 200-11	16.4	50
287	Towards improved local hybrid functionals by calibration of exchange-energy densities. *Journal of Chemical Physics*, **2014**, 141, 204101	3.9	49
286	Scalar relativistic calculations of hyperfine coupling tensors using the Douglas-Kroll-Hess method with a finite-size nucleus model. *Physical Chemistry Chemical Physics*, **2006**, 8, 4079-85	3.6	48
285	Relativistic Heavy-Neighbor-Atom Effects on NMR Shifts: Concepts and Trends Across the Periodic Table. *Chemical Reviews*, **2020**, 120, 7065-7103	68.1	47
284	Perturbational and ECP Calculation of Relativistic Effects in NMR Shielding and Spin-Spin Coupling **2004**, 209-226		47
283	Relativistic Effects on NMR Chemical Shifts. *Theoretical and Computational Chemistry*, **2004**, 14, 552-597		47
282	Ab Initio ECP/DFT Calculation and Interpretation of Carbon and Oxygen NMR Chemical Shift Tensors in Transition-Metal Carbonyl Complexes. *Chemistry - A European Journal*, **1996**, 2, 24-30	4.8	47
281	The Cluster Anion Si. *Angewandte Chemie - International Edition*, **1998**, 37, 2359-2361	16.4	46
280	Understanding structure and bonding in early actinide 6d(0)5f0 MX6q (M = Th-Np; X = H, F) complexes in comparison with their transition metal 5d0 analogues. *Journal of the American Chemical Society*, **2005**, 127, 2591-9	16.4	46
279	Pseudo-Contact NMR Shifts over the Paramagnetic Metalloprotein CoMMP-12 from First Principles. *Angewandte Chemie - International Edition*, **2016**, 55, 14713-14717	16.4	45

278	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, 10629-37	2.8	45
277	The Nonoctahedral Structures of d0, d1, and d2 Hexamethyl Complexes. *Chemistry - A European Journal*, **1998**, 4, 1678-1686	4.8	45
276	Structure of the nitrogen-centered radical formed during inactivation of E. coli ribonucleotide reductase by 2'-azido-2'-deoxyuridine-5'-diphosphate: trapping of the 3'-ketonucleotide. *Journal of the American Chemical Society*, **2005**, 127, 7729-38	16.4	45
275	Efficient Self-Consistent Implementation of Local Hybrid Functionals. *Journal of Chemical Theory and Computation*, **2015**, 11, 1540-8	6.4	44
274	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	16.4	44
273	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	5.4	43
272	What can we learn from the adiabatic connection formalism about local hybrid functionals?. *Journal of Chemical Physics*, **2008**, 128, 214107	3.9	43
271	Mercury Is a Transition Metal: The First Experimental Evidence for HgF4. *Angewandte Chemie*, **2007**, 119, 8523-8527	3.6	43
270	Formal Oxidation State versus Partial Charge—A Comment. *Angewandte Chemie International Edition in English*, **1995**, 34, 986-986		43
269	Solvent effects on g-tensors of semiquinone radical anions: polarizable continuum versus cluster models. *Theoretical Chemistry Accounts*, **2004**, 111, 132-140	1.9	42
268	New Zwitterionic Spirocyclic 5Si-Silicates with an SiX4C Skeleton (X = S, O) Containing Two Ligands of the Dithiolato(2)or Diolato(2)Type: Synthesis, Structure, and Bonding Situation. *Organometallics*, **2003**, 22, 4104-4110	3.8	42
267	ReSpect: Relativistic spectroscopy DFT program package. *Journal of Chemical Physics*, **2020**, 152, 184101	3.9	41
266	From Silylone to an Isolable Monomeric Silicon Disulfide Complex. *Angewandte Chemie - International Edition*, **2015**, 54, 10254-7	16.4	41
265	Local hybrid functionals with an explicit dependence on spin polarization. *Journal of Physical Chemistry A*, **2009**, 113, 11898-906	2.8	41
264	Construction of local hybrid exchange-correlation potentials and their evaluation for nuclear shielding constants. *Chemical Physics Letters*, **2004**, 386, 8-16	2.5	41
263	Advances in local hybrid exchange-correlation functionals: from thermochemistry to magnetic-resonance parameters and hyperpolarizabilities. *International Journal of Quantum Chemistry*, **2011**, 111, 2625-2638	2.1	40
262	First-Principles Calculations of Paramagnetic NMR Shifts **2004**, 325-338		40
261	Reaction of Pentadienyl Complexes with Metal Carbonyls: Synthetic, Structural, and Theoretical Studies of Metallabenzene Complexes. *Organometallics*, **2003**, 22, 264-274	3.8	40

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259	Efficient Semi-numerical Implementation of Global and Local Hybrid Functionals for Time-Dependent Density Functional Theory. *Journal of Chemical Theory and Computation*, **2015**, 11, 4226-37	6.4	39
258	Wavelength selective polymer network formation of end-functional star polymers. *Chemical Communications*, **2016**, 52, 1975-8	5.8	39
257	Diphosphines with strongly polarized P-P bonds: hybrids between covalent molecules and donor-acceptor adducts with flexible molecular structures. *Journal of the American Chemical Society* , **2009**, 131, 10763-74	16.4	39
256	In Situ Study on the Wet Chemical Synthesis of Nanoscopic Pt Colloids by □Reductive Stabilization□ *Journal of Physical Chemistry B*, **2003**, 107, 7507-7515	3.4	39
255	On the Relation between □Bonding, Electronegativity, and Bond Angles in High-Valent Transition Metal Complexes. *Chemistry - A European Journal*, **1999**, 5, 3631-3643	4.8	39
254	Four-Component Relativistic Density Functional Theory Calculations of EPR g- and Hyperfine-Coupling Tensors Using Hybrid Functionals: Validation on Transition-Metal Complexes with Large Tensor Anisotropies and Higher-Order Spin-Orbit Effects. *Journal of Physical Chemistry A* , **2015**, 119, 12892-905	2.8	38
253	Phosphorus chemical shifts in a nucleic acid backbone from combined molecular dynamics and density functional calculations. *Journal of the American Chemical Society*, **2010**, 132, 17139-48	16.4	38
252	□Unexpected□29Si NMR Chemical Shifts in Heteroatom-Substituted Silyllithium Compounds: A Quantum-Chemical Analysis. *Organometallics*, **2004**, 23, 3647-3655	3.8	38
251	gTensor and Spin Density of the Modified Tyrosyl Radical in Galactose Oxidase:□A Density Functional Study. *Journal of Physical Chemistry B*, **2003**, 107, 331-337	3.4	38
250	An Isolable Silicon Dicarbonate Complex from Carbon Dioxide Activation with a Silylone. *Angewandte Chemie - International Edition*, **2017**, 56, 1894-1897	16.4	37
249	A combined computational and spectroelectrochemical study of platinum-bridged bis-triarylamine systems. *Inorganic Chemistry*, **2014**, 53, 1544-54	5.1	37
248	Synthesis, structure, and reactivity of borole-functionalized ferrocenes. *Chemistry - A European Journal*, **2012**, 18, 11732-46	4.8	37
247	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	16.4	37
246	Insights into trans-Ligand and Spin-Orbit Effects on Electronic Structure and Ligand NMR Shifts in Transition-Metal Complexes. *Chemistry - A European Journal*, **2017**, 23, 9790-9803	4.8	36
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