Jochen Autschbach

List of Publications by Year
in descending order

		8732	17546
382	20,970	75	121
papers	citations	h-index	g-index

422	422	422	13751
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. Journal of Computational Chemistry, 2016, 37, 506-541.	1.5	1,317
2	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	2.3	661
3	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	1.2	425
4	Theoretical Methods of Potential Use for Studies of Inorganic Reaction Mechanisms. Chemical Reviews, 2005, 105, 2695-2722.	23.0	387
5	Chiroptical properties from time-dependent density functional theory. I. Circular dichroism spectra of organic molecules. Journal of Chemical Physics, 2002, 116, 6930-6940.	1.2	386
6	Computing chiroptical properties with firstâ€principles theoretical methods: Background and illustrative examples. Chirality, 2009, 21, E116-52.	1.3	296
7	Modern quantum chemistry with [Open]Molcas. Journal of Chemical Physics, 2020, 152, 214117.	1.2	281
8	Nuclear spinâ€“spin coupling constants from regular approximate relativistic density functional calculations. I. Formalism and scalar relativistic results for heavy metal compounds. Journal of Chemical Physics, 2000, 113, 936-947.	1.2	245
9	Delocalization Error and â€œFunctional Tuningâ€•in Kohnâ€“Sham Calculations of Molecular Properties. Accounts of Chemical Research, 2014, 47, 2592-2602.	7.6	239
10	Quasiparticle Spectra from a Nonempirical Optimally Tuned Range-Separated Hybrid Density Functional. Physical Review Letters, 2012, 109, 226405.	2.9	236
11	Perspective: Relativistic effects. Journal of Chemical Physics, 2012, 136, 150902.	1.2	234
12	Nuclear spinâ€“spin coupling constants from regular approximate relativistic density functional calculations. II. Spinâ€“orbit coupling effects and anisotropies. Journal of Chemical Physics, 2000, 113, 9410-9418.	1.2	208
13	Chargeâ€Transfer Excitations and Timeâ€Dependent Density Functional Theory: Problems and Some Proposed Solutions. ChemPhysChem, 2009, 10, 1757-1760.	1.0	190
14	Chiroptical properties from time-dependent density functional theory. II. Optical rotations of small to medium sized organic molecules. Journal of Chemical Physics, 2002, 117, 581-592.	1.2	186
15	Scope and Mechanistic Analysis of the Enantioselective Synthesis of Allenes by Rhodium-Catalyzed Tandem Ylide Formation/[2,3]-Sigmatropic Rearrangement between Donor/Acceptor Carbenoids and Propargylic Alcohols. Journal of the American Chemical Society, 2012, 134, 15497-15504.	6.6	177
16	Theory and method for calculating resonance Raman scattering from resonance polarizability derivatives. Journal of Chemical Physics, 2005, 123, 174110.	1.2	169
17	Computational Study on the Selectivity of Donor/Acceptor-Substituted Rhodium Carbenoids. Journal of Organic Chemistry, 2009, 74, 6555-6563.	1.7	169
18	Acid/Baseâ€Triggered Switching of Circularly Polarized Luminescence and Electronic Circular Dichroism in Organic and Organometallic Helicenes. Chemistry - A European Journal, 2015, 21, 1673-1681.	1.7	166

#	Article	IF	Citations
19	Direct Spectroscopic Characterization of a Transitory Dirhodium Donor-Acceptor Carbene Complex. Science, 2013, 342, 351-354.	6.0	165
20	Finite lifetime effects on the polarizability within time-dependent density-functional theory. Journal of Chemical Physics, 2005, 122, 224115.	1.2	161
21	Density Functional Calculations of the13C NMR Chemical Shifts in (9,0) Single-Walled Carbon Nanotubes. Journal of the American Chemical Society, 2004, 126, 13079-13088.	6.6	152
22	Curvature and Frontier Orbital Energies in Density Functional Theory. Journal of Physical Chemistry Letters, 2012, 3, 3740-3744.	2.1	145
23	Metallahelicenes: Easily Accessible Helicene Derivatives with Large and Tunable Chiroptical Properties. Angewandte Chemie - International Edition, 2010, 49, 99-102.	7.2	144
24	Enantiopure Cycloiridiated Complexes Bearing a Pentahelicenic Nâ€Heterocyclic Carbene and Displaying Longâ€Lived Circularly Polarized Phosphorescence. Angewandte Chemie - International Edition, 2017, 56, 8236-8239.	7.2	143
25	Electronic Energy Gaps for Ï€-Conjugated Oligomers and Polymers Calculated with Density Functional Theory. Journal of Chemical Theory and Computation, 2014, 10, 1035-1047.	2.3	142
26	Analysis of electric field gradient tensors at quadrupolar nuclei in common structural motifs. Concepts in Magnetic Resonance Part A: Bridging Education and Research, 2010, 36A, 84-126.	0.2	140
27	Does a Molecule-Specific Density Functional Give an Accurate Electron Density? The Challenging Case of the CuCl Electric Field Gradient. Journal of Physical Chemistry Letters, 2012, 3, 576-581.	2.1	140
28	Straightforward access to mono- and bis-cycloplatinated helicenes displaying circularly polarized phosphorescence by using crystallization resolution methods. Chemical Science, 2014, 5, 1915.	3.7	140
29	Performance of an Optimally Tuned Range-Separated Hybrid Functional for 0â€“0 Electronic Excitation Energies. Journal of Chemical Theory and Computation, 2014, 10, 1677-1685.	2.3	135
30	Chapter 1 Relativistic Computations of NMR Parameters from First Principles: Theory and Applications. Annual Reports on NMR Spectroscopy, 2009, 67, 1-95.	0.7	132
31	Metalâ^'Bis(helicene) Assemblies Incorporating Ï€-Conjugated Phosphole-Azahelicene Ligands: Impacting Chiroptical Properties by Metal Variation. Journal of the American Chemical Society, 2009, 131, 3183-3185.	6.6	127
32	Ruthenium-Vinylhelicenes: Remote Metal-Based Enhancement and Redox Switching of the Chiroptical Properties of a Helicene Core. Journal of the American Chemical Society, 2012, 134, 15628-15631.	6.6	126
33	Curing difficult cases in magnetic properties prediction with self-interaction corrected density functional theory. Journal of Chemical Physics, 2001, 115, 26-42.	1.2	125
34	Analyzing NMR shielding tensors calculated with two-component relativistic methods using spin-free localized molecular orbitals. Journal of Chemical Physics, 2008, 128, 164112.	1.2	125
35	Exciton coupling in diketopyrrolopyrroleâ€“helicene derivatives leads to red and near-infrared circularly polarized luminescence. Chemical Science, 2018, 9, 735-742.	3.7	122
36	Influence of the Delocalization Error and Applicability of Optimal Functional Tuning in Density Functional Calculations of Nonlinear Optical Properties of Organic Donorâ€“Acceptor Chromophores. ChemPhysChem, 2013, 14, 2450-2461.	1.0	119

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37	Analyzing Pt chemical shifts calculated from relativistic density functional theory using localized orbitals: The role of Pt 5d lone pairs. Magnetic Resonance in Chemistry, 2008, 46, S45-S55.	1.1	118
38	Calculating Natural Optical Activity of Molecules from First Principles. Annual Review of Physical Chemistry, 2017, 68, 399-420.	4.8	117
39	Rhodium(II)â€Catalyzed Crossâ€Coupling of Diazo Compounds. Angewandte Chemie - International Edition, 2011, 50, 2544-2548.	7.2	114
40	Assessing the exchange coupling in binuclear lanthanide(<scp>iii</scp>) complexes and the slow relaxation of the magnetization in the antiferromagnetically coupled Dy₂ derivative. Chemical Science, 2015, 6, 4148-4159.	3.7	114
41	Optical Rotation Calculated with Time-Dependent Density Functional Theory: The OR45 Benchmark. Journal of Physical Chemistry A, 2011, 115, 10930-10949.	1.1	110
42	Tuned Range-Separated Time-Dependent Density Functional Theory Applied to Optical Rotation. Journal of Chemical Theory and Computation, 2012, 8, 245-256.	2.3	109
43	Highly Enantioselective Rh₂(S-DOSP)₄-Catalyzed Cyclopropenation of Alkynes with Styryldiazoacetates. Journal of the American Chemical Society, 2010, 132, 17211-17215.	6.6	108
44	Calculation of Hyperfine Tensors and Paramagnetic NMR Shifts Using the Relativistic Zeroth-Order Regular Approximation and Density Functional Theory. Journal of Chemical Theory and Computation, 2011, 7, 2175-2188.	2.3	107
45	Longest-Wavelength Electronic Excitations of Linear Cyanines: The Role of Electron Delocalization and of Approximations in Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2013, 9, 4991-5003.	2.3	107
46	Achieving high circularly polarized luminescence with pushâ€“pull helicenic systems: from rationalized design to top-emission CP-OLED applications. Chemical Science, 2021, 12, 5522-5533.	3.7	106
47	Magnitude of Zero-Point Vibrational Corrections to Optical Rotation in Rigid Organic Molecules:Â A Time-Dependent Density Functional Study. Journal of Physical Chemistry A, 2005, 109, 8617-8623.	1.1	104
48	Synthesis and Chiroptical Properties of Hexaâ€, Octaâ€, and Decaâ€azaborahelicenes: Influence of Helicene Size and of the Number of Boron Atoms. Chemistry - A European Journal, 2017, 23, 407-418.	1.7	102
49	Calculating molecular electric and magnetic properties from time-dependent density functional response theory. Journal of Chemical Physics, 2002, 116, 891-896.	1.2	101
50	Double perturbation theory: a powerful tool in computational coordination chemistry. Coordination Chemistry Reviews, 2003, 238-239, 83-126.	9.5	101
51	Dependence of relativistic effects on electronic configuration in the neutral atoms of d- and f-block elements. Journal of Computational Chemistry, 2002, 23, 804-813.	1.5	99
52	Time-Dependent Density Functional Response Theory for Electronic Chiroptical Properties of Chiral Molecules. Topics in Current Chemistry, 2010, 298, 1-98.	4.0	98
53	Properties of WAu12. Physical Chemistry Chemical Physics, 2004, 6, 11-22.	1.3	97
54	On the relation between time-dependent and variational density functional theory approaches for the determination of excitation energies and transition moments.. Journal of Chemical Physics, 2009, 130, 154102.	1.2	96

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55	Calculation of optical rotation with time-periodic magnetic-field-dependent basis functions in approximate time-dependent density-functional theory. Journal of Chemical Physics, 2005, 123, 114103.	1.2	92
56	On the Mechanism and Selectivity of the Combined Câ^'H Activation/Cope Rearrangement. Journal of the American Chemical Society, 2011, 133, 5076-5085.	6.6	92
57	Density Functional Calculations on Electronic Circular Dichroism Spectra of Chiral Transition Metal Complexes. Inorganic Chemistry, 2003, 42, 2867-2877.	1.9	91
58	enantio-Enriched CPL-active heliceneâ€"bipyridineâ€"rhenium complexes. Chemical Communications, 2015, 51, 3754-3757.	2.2	91
59	Density functional theory applied to calculating optical and spectroscopic properties of metal complexes: NMR and optical activity. Coordination Chemistry Reviews, 2007, 251, 1796-1821.	9.5	87
60	Scalar Relativistic Computations and Localized Orbital Analyses of Nuclear Hyperfine Coupling and Paramagnetic NMR Chemical Shifts. Journal of Chemical Theory and Computation, 2012, 8, 598-609.	2.3	87
61	Characterization of berkelium(III) dipicolinate and borate compounds in solution and the solid state. Science, 2016, 353, .	6.0	86
62	Solid-State Chlorine NMR of Group IV Transition Metal Organometallic Complexes. Journal of the American Chemical Society, 2009, 131, 3317-3330.	6.6	85
63	Magnetic Properties and Electronic Structure of Neptunyl(VI) Complexes: Wavefunctions, Orbitals, and Crystalâ€Field Models. Chemistry - A European Journal, 2014, 20, 7994-8011.	1.7	85
64	Accurate dipole polarizabilities for water clusters n=2â€"12 at the coupled-cluster level of theory and benchmarking of various density functionals. Journal of Chemical Physics, 2009, 131, 214103.	1.2	83
65	The role of the exchange-correlation response kernel and scaling corrections in relativistic density functional nuclear magnetic shielding calculations with the zeroth-order regular approximation. Molecular Physics, 2013, 111, 2544-2554.	0.8	83
66	Conformational changes and chiroptical switching of enantiopure bis-helicenic terpyridine upon Zn²⁺ binding. Chemical Communications, 2016, 52, 5932-5935.	2.2	83
67	Enantioselective Recognition of Ammonium Carbamates in a Chiral Metalâ€"Organic Framework. Journal of the American Chemical Society, 2017, 139, 16000-16012.	6.6	82
68	On the Origin of Optical Activity in Tris-diamine Complexes of Co(III) and Rh(III):Â A Simple Model Based on Time-Dependent Density Function Theory. Journal of the American Chemical Society, 2005, 127, 975-985.	6.6	79
69	Assembly of Ï€â€Conjugated Phosphole Azahelicene Derivatives into Chiral Coordination Complexes: An Experimental and Theoretical Study. Chemistry - A European Journal, 2010, 16, 5976-6005.	1.7	79
70	Applications of Time Dependent and Time Independent Density Functional Theory to the First Ï€ to Ï€* Transition in Cyanine Dyes. Journal of Chemical Theory and Computation, 2014, 10, 3299-3307.	2.3	79
71	Modulation of circularly polarized luminescence through excited-state symmetry breaking and interbranched exciton coupling in helical pushâ€"pull organic systems. Chemical Science, 2020, 11, 567-576.	3.7	79
72	Solvent Effects on Heavy Atom Nuclear Spinâ^'Spin Coupling Constants:Â A Theoretical Study of Hgâ^'C and Ptâ^'P Couplings. Journal of the American Chemical Society, 2001, 123, 3341-3349.	6.6	78

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73	Resonance vibrational Raman optical activity: A time-dependent density functional theory approach. Journal of Chemical Physics, 2007, 127, 134101.	1.2	78
74	From Hetero- to Homochiral Bis(metallahelicene)s Based on a Pt^{III}â^'Pt^{III} Bonded Scaffold: Isomerization, Structure, and Chiroptical Properties. Journal of the American Chemical Society, 2011, 133, 3800-3803.	6.6	78
75	Interaction Tensors and Local Dynamics in Common Structural Motifs of Nitrogen: A Solid-State ¹⁴N NMR and DFT Study. Journal of the American Chemical Society, 2011, 133, 527-546.	6.6	77
76	Timeâ€Dependent Density Functional Theory for Calculating Originâ€Independent Optical Rotation and Rotatory Strength Tensors. ChemPhysChem, 2011, 12, 3224-3235.	1.0	77
77	Tellurium Analogues of Rosamine and Rhodamine Dyes:â€‰ Synthesis, Structure, 125Te NMR, and Heteroatom Contributions to Excitation Energies. Organometallics, 2007, 26, 6248-6257.	1.1	76
78	The Calculation of NMR Parameters in Transition Metal Complexes. Structure and Bonding, 2004, , 1-48.	1.0	75
79	Charge-Transfer Versus Charge-Transfer-Like Excitations Revisited. Journal of Chemical Theory and Computation, 2015, 11, 3305-3320.	2.3	75
80	Magnitude of Finiteâ€Nucleusâ€Size Effects in Relativistic Density Functional Computations of Indirect NMR Nuclear Spinâ€“Spin Coupling Constants. ChemPhysChem, 2009, 10, 2274-2283.	1.0	74
81	Time-Dependent Density Functional Calculations of Optical Rotatory Dispersion Including Resonance Wavelengths as a Potentially Useful Tool for Determining Absolute Configurations of Chiral Molecules. Journal of Physical Chemistry A, 2006, 110, 2461-2473.	1.1	72
82	Analyzing and Interpreting NMR Spinâ€“Spin Coupling Constants Using Molecular Orbital Calculations. Journal of Chemical Education, 2007, 84, 156.	1.1	71
83	²⁹Si DFT/NMR Observation of Spinâ€“Orbit Effect in Metallasilatrane Sheds Some Light on the Strength of the Metalâ†'Silicon Interaction. Angewandte Chemie - International Edition, 2011, 50, 255-259.	7.2	71
84	Iron Alkynyl Helicenes: Redoxâ€Triggered Chiroptical Tuning in the IR and Nearâ€IR Spectral Regions and Suitable for Telecommunications Applications. Angewandte Chemie - International Edition, 2016, 55, 8062-8066.	7.2	71
85	Relativistic Density-Functional Computations of the Chemical Shift of129Xe in Xe@C60. Journal of Physical Chemistry A, 2003, 107, 4967-4972.	1.1	70
86	Toward an Accurate Determination of 195Pt Chemical Shifts by Density Functional Computations:â€‰ The Importance of Unspecific Solvent Effects and the Dependence of Pt Magnetic Shielding Constants on Structural Parameters. Inorganic Chemistry, 2006, 45, 3316-3324.	1.9	69
87	Relativistic calculations of magnetic resonance parameters: background and some recent developments. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20120489.	1.6	68
88	Calculation of origin-independent optical rotation tensor components in approximate time-dependent density functional theory. Journal of Chemical Physics, 2006, 125, 034102.	1.2	67
89	Temperature dependence of contact and dipolar NMR chemical shifts in paramagnetic molecules. Journal of Chemical Physics, 2015, 142, 054108.	1.2	67
90	Two-component relativistic hybrid density functional computations of nuclear spin-spin coupling tensors using Slater-type basis sets and density-fitting techniques. Journal of Chemical Physics, 2008, 129, 094105.	1.2	66

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91	A revised electronic Hessian for approximate time-dependent density functional theory. Journal of Chemical Physics, 2008, 129, 184114.	1.2	65
92	Probing the Solvent Shell with 195Pt Chemical Shifts: Density Functional Theory Molecular Dynamics Study of PtII and PtIV Anionic Complexes in Aqueous Solution. Journal of the American Chemical Society, 2010, 132, 3472-3483.	6.6	65
93	Unravelling the Structure of Magnusâ€™ Pink Salt. Journal of the American Chemical Society, 2014, 136, 1333-1351.	6.6	65
94	A Theoretical Investigation of the Remarkable Nuclear Spinâ^'Spin Coupling Pattern in [(NC)5Ptâ^'Tl(CN)]-. Journal of the American Chemical Society, 2001, 123, 5320-5324.	6.6	64
95	Calculation of molecular g-tensors using the zeroth-order regular approximation and density functional theory: expectation value versus linear response approaches. Theoretical Chemistry Accounts, 2011, 129, 453-466.	0.5	64
96	Calculating NMR Chemical Shifts for Paramagnetic Metal Complexes from First-Principles. Journal of Physical Chemistry Letters, 2015, 6, 2183-2188.	2.1	64
97	Longâ€Lived Circularly Polarized Phosphorescence in Heliceneâ€NHC Rhenium(I) Complexes: The Influence of Helicene, Halogen, and Stereochemistry on Emission Properties. Angewandte Chemie - International Edition, 2020, 59, 8394-8400.	7.2	64
98	A diuranium carbide cluster stabilized inside a C80 fullerene cage. Nature Communications, 2018, 9, 2753.	5.8	63
99	Density Functional Study of the 13C NMR Chemical Shifts in Small-to-Medium-Diameter Infinite Single-Walled Carbon Nanotubes. Journal of Physical Chemistry A, 2006, 110, 11995-12004.	1.1	62
100	Relativistic Zeroth-Order Regular Approximation Combined with Nonhybrid and Hybrid Density Functional Theory: Performance for NMR Indirect Nuclear Spinâ^'Spin Coupling in Heavy Metal Compounds. Journal of Chemical Theory and Computation, 2010, 6, 223-234.	2.3	62
101	Multifunctional and Reactive Enantiopure Organometallic Helicenes: Tuning Chiroptical Properties by Structural Variations of Monoâ€and Bis(platinahelicene)s. Chemistry - A European Journal, 2011, 17, 14178-14198.	1.7	62
102	Two-Component Relativistic Calculations of Electric-Field Gradients Using Exact Decoupling Methods: Spinâ€“orbit and Picture-Change Effects. Journal of Chemical Theory and Computation, 2012, 8, 4239-4248.	2.3	62
103	Combined Experimental and Computational Studies of Heterobimetallic Biâ^'Rh Paddlewheel Carboxylates as Catalysts for Metal Carbenoid Transformations. Journal of Organic Chemistry, 2009, 74, 6564-6571.	1.7	61
104	Calculation of the Vibrationally Resolved, Circularly Polarized Luminescence of dâ€Camphorquinone and (S,S)â€transâ€²â€Hydrindanone. ChemPhysChem, 2010, 11, 2409-2415.	3.0	60
105	Solvent Effects and Dynamic Averaging of ¹⁹⁵Pt NMR Shielding in Cisplatin Derivatives. Inorganic Chemistry, 2011, 50, 1723-1732.	1.9	60
106	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.	1.9	60
107	Understanding and Controlling the Emission Brightness and Color of Molecular Cerium Luminophores. Journal of the American Chemical Society, 2018, 140, 4588-4595.	6.6	60
108	The roles of 4f- and 5f-orbitals in bonding: a magnetochemical, crystal field, density functional theory, and multi-reference wavefunction study. Dalton Transactions, 2016, 45, 11508-11521.	1.6	59

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109	Calculation of the A term of magnetic circular dichroism based on time dependent-density functional theory I. Formulation and implementation. Journal of Chemical Physics, 2004, 120, 10942-10954.	1.2	58
110	Transuranic Hybrid Materials: Crystallographic and Computational Metrics of Supramolecular Assembly. Journal of the American Chemical Society, 2017, 139, 10843-10855.	6.6	58
111	Calculation of Verdet constants with time-dependent density functional theory: Implementation and results for small molecules. Journal of Chemical Physics, 2005, 122, 074105.	1.2	57
112	Calculation of circular dichroism spectra from optical rotatory dispersion, and vice versa, as complementary tools for theoretical studies of optical activity using time-dependent density functional theory. Journal of Chemical Physics, 2006, 125, 194110.	1.2	57
113	Density Functional Calculation of the Electronic Circular Dichroism Spectra of the Transition Metal Complexes [M(phen)3]2+(M = Fe, Ru, Os). Journal of Physical Chemistry A, 2005, 109, 4836-4846.	1.1	56
114	Density Functional Study of the ¹³C NMR Chemical Shifts in Single-Walled Carbon Nanotubes with Stoneâ^'Wales Defects. Journal of Physical Chemistry C, 2008, 112, 11744-11750.	1.5	56
115	Is charge transfer transitions really too difficult for standard density functionals or are they just a problem for time-dependent density functional theory based on a linear response approach. Computational and Theoretical Chemistry, 2009, 914, 106-109.	1.5	56
116	Enhancement of IR and VCD intensities due to charge transfer. Physical Chemistry Chemical Physics, 2009, 11, 1526.	1.3	56
117	Theoretical Investigation of Paramagnetic NMR Shifts in Transition Metal Acetylacetonato Complexes: Analysis of Signs, Magnitudes, and the Role of the Covalency of Ligandâ€"Metal Bonding. Inorganic Chemistry, 2012, 51, 8340-8351.	1.9	56
118	Periodic Trends in Indirect Nuclear Spinâ^'Spin Coupling Tensors:â€‰ Relativistic Density Functional Calculations for Interhalogen Diatomics. Journal of the American Chemical Society, 2002, 124, 4894-4900.	6.6	54
119	Importance of vibronic effects on the circular dichroism spectrum of dimethyloxirane. Journal of Chemical Physics, 2005, 122, 234305.	1.2	54
120	Analyzing molecular properties calculated with two-component relativistic methods using spin-free natural bond orbitals: NMR spin-spin coupling constants. Journal of Chemical Physics, 2007, 127, 124106.	1.2	54
121	Analysis of Optical Activity in Terms of Bonds and Lone-Pairs: The Exceptionally Large Optical Rotation of Norbornenone. Journal of Chemical Theory and Computation, 2012, 8, 4336-4346.	2.3	54
122	Spectral and Structural Characterization of Amidate-Bridged Platinumâ^'Thallium Complexes with Strong Metalâ^'Metal Bonds. Inorganic Chemistry, 2006, 45, 4526-4536.	1.9	53
123	Computational Modeling of Polyoxotungstates by Relativistic DFT Calculations of183W NMR Chemical Shifts. Chemistry - A European Journal, 2006, 12, 8460-8471.	1.7	53
124	Atomic Contributions from Spinâ€Orbit Coupling to ²⁹Si NMR Chemical Shifts in Metallasilatrane Complexes. Chemistry - A European Journal, 2012, 18, 12803-12813.	1.7	53
125	Single-ion 4f element magnetism: an ab-initio look at Ln(COT)₂^{â^'}. Dalton Transactions, 2015, 44, 19886-19900.	1.6	52
126	Calculation of static and dynamic linear magnetic response in approximate time-dependent density functional theory. Journal of Chemical Physics, 2007, 126, 024101.	1.2	50

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127	A quantum chemical approach to the design of chiral negative index materials. Optics Express, 2007, 15, 5730.	1.7	50
128	Variational versus Perturbational Treatment of Spinâ€“Orbit Coupling in Relativistic Density Functional Calculations of Electronic g Factors: Effects from Spin-Polarization and Exact Exchange. Journal of Chemical Theory and Computation, 2013, 9, 1052-1067.	2.3	50
129	On the Origin of the Optical Activity in the dâ^'d Transition Region of Tris-Bidentate Co(III) and Rh(III) Complexes. Inorganic Chemistry, 2003, 42, 8902-8910.	1.9	49
130	Magnetic Resonance Properties of Actinyl Carbonate Complexes and Plutonyl(VI)-tris-nitrate. Inorganic Chemistry, 2014, 53, 8577-8592.	1.9	49
131	Impact of the Kohnâ€“Sham Delocalization Error on the 4f Shell Localization and Population in Lanthanide Complexes. Journal of Chemical Theory and Computation, 2016, 12, 3109-3121.	2.3	49
132	Calculation of the magnetic circular dichroism B term from the imaginary part of the Verdet constant using damped time-dependent density functional theory. Journal of Chemical Physics, 2007, 127, 244102.	1.2	48
133	Time Dependent Density Functional Theory Modeling of Chiroptical Properties of Small Amino Acids in Solution. Journal of Physical Chemistry A, 2006, 110, 4115-4123.	1.1	47
134	A Density Functional Study of the13C NMR Chemical Shifts in Functionalized Single-Walled Carbon Nanotubes. Journal of the American Chemical Society, 2007, 129, 4430-4439.	6.6	47
135	Ab Initio and Density Functional Theory Modeling of the Chiroptical Response of Glycine and Alanine in Solution Using Explicit Solvation and Molecular Dynamics. Journal of Chemical Theory and Computation, 2008, 4, 1902-1914.	2.3	47
136	Electric Field Gradients Calculated from Two-Component Hybrid Density Functional Theory Including Spinâ^'Orbit Coupling. Journal of Chemical Theory and Computation, 2010, 6, 2669-2686.	2.3	47
137	A Theoretical Study of the NMR Spinâ^'Spin Coupling Constants of the Complexes [(NC)5Ptâ^'Tl(CN)n]n-(n= 0â^'3) and [(NC)5Ptâ^'Tlâ^'Pt(CN)5]3-:Â A Lesson on Environmental Effects. Journal of the American Chemical Society, 2003, 125, 13585-13593.	6.6	46
138	Application of magnetically perturbed time-dependent density functional theory to magnetic circular dichroism: Calculation of B terms. Journal of Chemical Physics, 2008, 128, 144105.	1.2	46
139	Modeling of the Chiroptical Response of Chiral Amino Acids in Solution Using Explicit Solvation and Molecular Dynamics. Journal of Chemical Theory and Computation, 2009, 5, 1051-1060.	2.3	46
140	Orbitals: Some Fiction and Some Facts. Journal of Chemical Education, 2012, 89, 1032-1040.	1.1	46
141	Relativistic Density Functional Calculations of Hyperfine Coupling with Variational versus Perturbational Treatment of Spinâ€“Orbit Coupling. Journal of Chemical Theory and Computation, 2013, 9, 1932-1948.	2.3	46
142	Engaging the Terminal: Promoting Halogen Bonding Interactions with Uranyl Oxo Atoms. Chemistry - A European Journal, 2017, 23, 15355-15369.	1.7	46
143	Use of ¹⁵N NMR spectroscopy to probe covalency in a thorium nitride. Chemical Science, 2019, 10, 6431-6436.	3.7	46
144	The accuracy of hyperfine integrals in relativistic NMR computations based on the zeroth-order regular approximation. Theoretical Chemistry Accounts, 2004, 112, 52-57.	0.5	45

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145	NMR properties of platinumï£¿thallium bonded complexes: analysis of relativistic density functional theory results. Magnetic Resonance in Chemistry, 2004, 42, S99-S116.	1.1	45
146	Solvent Effects on195Pt and205Tl NMR Chemical Shifts of the Complexes[(NC)5Ptï£¿Tl(CN)n]nâ^' (n=0â€“3), and[(NC)5Ptï£¿Tlï£¿Pt(CN)5]3â^' Studied by Relativistic Density Functional Theory. Chemistry - A European Journal, 2004, 10, 2581-2589.	1.7	45
147	Application of magnetically perturbed time-dependent density functional theory to magnetic circular dichroism. II. Calculation of A terms. Journal of Chemical Physics, 2008, 128, 234102.	1.2	45
148	Theoretical studies of surface enhanced hyper-Raman spectroscopy: The chemical enhancement mechanism. Journal of Chemical Physics, 2010, 133, 054103.	1.2	45
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