Jochen Autschbach

List of Publications by Citations

376 papers	16,871 citations	69 h-index	108 g-index
422 ext. papers	19,071 ext. citations	6.4 avg, IF	7.21 L-index

#	Paper	IF	Citations
376	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, **2016**, 37, 506-41	3.5	1047
375	Theoretical methods of potential use for studies of inorganic reaction mechanisms. *Chemical Reviews*, **2005**, 105, 2695-722	68.1	364
374	Chiroptical properties from time-dependent density functional theory. I. Circular dichroism spectra of organic molecules. *Journal of Chemical Physics*, **2002**, 116, 6930-6940	3.9	346
373	OpenMolcas: From Source Code to Insight. *Journal of Chemical Theory and Computation*, **2019**, 15, 5925-5964	5.4	310
372	Computing chiroptical properties with first-principles theoretical methods: background and illustrative examples. *Chirality*, **2009**, 21 Suppl 1, E116-52	2.1	264
371	Nuclear spin–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	3.9	218
370	Quasiparticle spectra from a nonempirical optimally tuned range-separated hybrid density functional. *Physical Review Letters*, **2012**, 109, 226405	7.4	203
369	Delocalization error and "functional tuning" in Kohn-Sham calculations of molecular properties. *Accounts of Chemical Research*, **2014**, 47, 2592-602	24.3	196
368	Perspective: relativistic effects. *Journal of Chemical Physics*, **2012**, 136, 150902	3.9	189
367	Nuclear spin–spin coupling constants from regular approximate relativistic density functional calculations. II. Spin–orbit coupling effects and anisotropies. *Journal of Chemical Physics*, **2000**, 113, 9410-9418	3.9	189
366	NWChem: Past, present, and future. *Journal of Chemical Physics*, **2020**, 152, 184102	3.9	187
365	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	3.9	168
364	Charge-transfer excitations and time-dependent density functional theory: problems and some proposed solutions. *ChemPhysChem*, **2009**, 10, 1757-60	3.2	167
363	Theory and method for calculating resonance Raman scattering from resonance polarizability derivatives. *Journal of Chemical Physics*, **2005**, 123, 174110	3.9	155
362	Computational study on the selectivity of donor/acceptor-substituted rhodium carbenoids. *Journal of Organic Chemistry*, **2009**, 74, 6555-63	4.2	154
361	Density functional calculations of the 13C NMR chemical shifts in (9,0) single-walled carbon nanotubes. *Journal of the American Chemical Society*, **2004**, 126, 13079-88	16.4	148
360	Direct spectroscopic characterization of a transitory dirhodium donor-acceptor carbene complex. *Science*, **2013**, 342, 351-4	33.3	146

359	Finite lifetime effects on the polarizability within time-dependent density-functional theory. *Journal of Chemical Physics*, **2005**, 122, 224115	3.9	146
358	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, 15497-504	16.4	143
357	Curvature and Frontier Orbital Energies in Density Functional Theory. *Journal of Physical Chemistry Letters*, **2012**, 3, 3740-4	6.4	134
356	Acid/base-triggered switching of circularly polarized luminescence and electronic circular dichroism in organic and organometallic helicenes. *Chemistry - A European Journal*, **2015**, 21, 1673-81	4.8	126
355	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, 576-81	6.4	126
354	Metallahelicenes: easily accessible helicene derivatives with large and tunable chiroptical properties. *Angewandte Chemie - International Edition*, **2010**, 49, 99-102	16.4	126
353	Metal-bis(helicene) assemblies incorporating pi-conjugated phosphole-azahelicene ligands: impacting chiroptical properties by metal variation. *Journal of the American Chemical Society*, **2009**, 131, 3183-5	16.4	120
352	Curing difficult cases in magnetic properties prediction with self-interaction corrected density functional theory. *Journal of Chemical Physics*, **2001**, 115, 26-42	3.9	118
351	Chapter 1 Relativistic Computations of NMR Parameters from First Principles: Theory and Applications. *Annual Reports on NMR Spectroscopy*, **2009**, 67, 1-95	1.7	115
350	Performance of an Optimally Tuned Range-Separated Hybrid Functional for 0-0 Electronic Excitation Energies. *Journal of Chemical Theory and Computation*, **2014**, 10, 1677-85	6.4	113
349	Electronic Energy Gaps for π-Conjugated Oligomers and Polymers Calculated with Density Functional Theory. *Journal of Chemical Theory and Computation*, **2014**, 10, 1035-47	6.4	111
348	Enantiopure Cycloiridiated Complexes Bearing a Pentahelicenic N-Heterocyclic Carbene and Displaying Long-Lived Circularly Polarized Phosphorescence. *Angewandte Chemie - International Edition*, **2017**, 56, 8236-8239	16.4	110
347	Influence of the delocalization error and applicability of optimal functional tuning in density functional calculations of nonlinear optical properties of organic donor-acceptor chromophores. *ChemPhysChem*, **2013**, 14, 2450-61	3.2	110
346	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	0.6	110
345	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, 15628-31	16.4	108
344	Modern quantum chemistry with [Open]Molcas. *Journal of Chemical Physics*, **2020**, 152, 214117	3.9	106
343	Analyzing NMR shielding tensors calculated with two-component relativistic methods using spin-free localized molecular orbitals. *Journal of Chemical Physics*, **2008**, 128, 164112	3.9	106
342	Assessing the exchange coupling in binuclear lanthanide(iii) complexes and the slow relaxation of the magnetization in the antiferromagnetically coupled Dy derivative. *Chemical Science*, **2015**, 6, 4148-4159	8.4	102

341	Straightforward access to mono- and bis-cycloplatinated helicenes that display circularly polarized phosphorescence using crystallization resolution methods. *Chemical Science*, **2014**, 5, 1915-1927	9.4	99
340	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 Suppl 1, S45-55	2.1	98
339	Optical rotation calculated with time-dependent density functional theory: the OR45 benchmark. *Journal of Physical Chemistry A*, **2011**, 115, 10930-49	2.8	97
338	Highly enantioselective Rh2(S-DOSP)4-catalyzed cyclopropenation of alkynes with styryldiazoacetates. *Journal of the American Chemical Society*, **2010**, 132, 17211-5	16.4	97
337	Magnitude of zero-point vibrational corrections to optical rotation in rigid organic molecules: a time-dependent density functional study. *Journal of Physical Chemistry A*, **2005**, 109, 8617-23	2.8	97
336	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	6.4	96
335	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, 2175-88	6.4	93
334	Properties of WAu12. *Physical Chemistry Chemical Physics*, **2004**, 6, 11-22	3.6	93
333	Tuned Range-Separated Time-Dependent Density Functional Theory Applied to Optical Rotation. *Journal of Chemical Theory and Computation*, **2012**, 8, 245-56	6.4	92
332	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	3.9	90
331	Dependence of relativistic effects on electronic configuration in the neutral atoms of d- and f-block elements. *Journal of Computational Chemistry*, **2002**, 23, 804-13	3.5	89
330	Calculating Natural Optical Activity of Molecules from First Principles. *Annual Review of Physical Chemistry*, **2017**, 68, 399-420	15.7	88
329	Rhodium(II)-catalyzed cross-coupling of diazo compounds. *Angewandte Chemie - International Edition*, **2011**, 50, 2544-8	16.4	87
328	Double perturbation theory: a powerful tool in computational coordination chemistry. *Coordination Chemistry Reviews*, **2003**, 238-239, 83-126	23.2	86
327	Density functional calculations on electronic circular dichroism spectra of chiral transition metal complexes. *Inorganic Chemistry*, **2003**, 42, 2867-77	5.1	86
326	Calculating molecular electric and magnetic properties from time-dependent density functional response theory. *Journal of Chemical Physics*, **2002**, 116, 891-896	3.9	86
325	Time-dependent density functional response theory for electronic chiroptical properties of chiral molecules. *Topics in Current Chemistry*, **2011**, 298, 1-98		84
324	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	3.9	83

323	Exciton coupling in diketopyrrolopyrrole-helicene derivatives leads to red and near-infrared circularly polarized luminescence. *Chemical Science*, **2018**, 9, 735-742	9.4	82
322	On the mechanism and selectivity of the combined C-H activation/Cope rearrangement. *Journal of the American Chemical Society*, **2011**, 133, 5076-85	16.4	81
321	Solid-state chlorine NMR of group IV transition metal organometallic complexes. *Journal of the American Chemical Society*, **2009**, 131, 3317-30	16.4	79
320	Accurate dipole polarizabilities for water clusters n=2-12 at the coupled-cluster level of theory and benchmarking of various density functionals. *Journal of Chemical Physics*, **2009**, 131, 214103	3.9	78
319	Density functional theory applied to calculating optical and spectroscopic properties of metal complexes: NMR and optical activity. *Coordination Chemistry Reviews*, **2007**, 251, 1796-1821	23.2	76
318	From hetero- to homochiral bis(metallahelicene)s based on a Pt(III)-Pt(III) bonded scaffold: isomerization, structure, and chiroptical properties. *Journal of the American Chemical Society*, **2011**, 133, 3800-3	16.4	75
317	Assembly of pi-conjugated phosphole azahelicene derivatives into chiral coordination complexes: an experimental and theoretical study. *Chemistry - A European Journal*, **2010**, 16, 5976-6005	4.8	75
316	Characterization of berkelium(III) dipicolinate and borate compounds in solution and the solid state. *Science*, **2016**, 353,	33.3	73
315	Magnetic properties and electronic structure of neptunyl(VI) complexes: wavefunctions, orbitals, and crystal-field models. *Chemistry - A European Journal*, **2014**, 20, 7994-8011	4.8	73
314	Applications of Time Dependent and Time Independent Density Functional Theory to the First □to □ Transition in Cyanine Dyes. *Journal of Chemical Theory and Computation*, **2014**, 10, 3299-307	6.4	73
313	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, 527-46	16.4	73
312	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	6.4	72
311	On the origin of optical activity in tris-diamine complexes of Co(III) and Rh(III): a simple model based on time-dependent density function theory. *Journal of the American Chemical Society*, **2005**, 127, 975-85	16.4	71
310	enantio-Enriched CPL-active helicene-bipyridine-rhenium complexes. *Chemical Communications*, **2015**, 51, 3754-7	5.8	70
309	(29)Si DFT/NMR observation of spin-orbit effect in metallasilatrane sheds some light on the strength of the metal-silicon interaction. *Angewandte Chemie - International Edition*, **2011**, 50, 255-9	16.4	70
308	Conformational changes and chiroptical switching of enantiopure bis-helicenic terpyridine upon Zn(2+) binding. *Chemical Communications*, **2016**, 52, 5932-5	5.8	69
307	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, 2461-73	2.8	69
306	Solvent effects on heavy atom nuclear spin-spin coupling constants: a theoretical study of Hg-C and Pt-P couplings. *Journal of the American Chemical Society*, **2001**, 123, 3341-9	16.4	69

305	Synthesis and Chiroptical Properties of Hexa-, Octa-, and Deca-azaborahelicenes: Influence of Helicene Size and of the Number of Boron Atoms. *Chemistry - A European Journal*, **2017**, 23, 407-418	4.8	68
304	Resonance vibrational Raman optical activity: a time-dependent density functional theory approach. *Journal of Chemical Physics*, **2007**, 127, 134101	3.9	68
303	Magnitude of finite-nucleus-size effects in relativistic density functional computations of indirect NMR nuclear spin-spin coupling constants. *ChemPhysChem*, **2009**, 10, 2274-83	3.2	64
302	Toward an accurate determination of 195Pt chemical shifts by density functional computations: the importance of unspecific solvent effects and the dependence of Pt magnetic shielding constants on structural parameters. *Inorganic Chemistry*, **2006**, 45, 3316-24	5.1	64
301	The Calculation of NMR Parameters in Transition Metal Complexes. *Structure and Bonding*, **2004**, 1-48	0.9	64
300	Charge-Transfer Versus Charge-Transfer-Like Excitations Revisited. *Journal of Chemical Theory and Computation*, **2015**, 11, 3305-20	6.4	62
299	A revised electronic Hessian for approximate time-dependent density functional theory. *Journal of Chemical Physics*, **2008**, 129, 184114	3.9	62
298	Tellurium Analogues of Rosamine and Rhodamine Dyes: Synthesis, Structure, 125Te NMR, and Heteroatom Contributions to Excitation Energies. *Organometallics*, **2007**, 26, 6248-6257	3.8	62
297	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, 11995-2004	2.8	62
296	Enantioselective Recognition of Ammonium Carbamates in a Chiral Metal-Organic Framework. *Journal of the American Chemical Society*, **2017**, 139, 16000-16012	16.4	61
295	Analyzing and Interpreting NMR Spin–Spin Coupling Constants Using Molecular Orbital Calculations. *Journal of Chemical Education*, **2007**, 84, 156	2.4	61
294	Time-dependent density functional theory for calculating origin-independent optical rotation and rotatory strength tensors. *ChemPhysChem*, **2011**, 12, 3224-35	3.2	60
293	Probing the solvent shell with 195Pt chemical shifts: density functional theory molecular dynamics study of Pt(II) and Pt(IV) anionic complexes in aqueous solution. *Journal of the American Chemical Society*, **2010**, 132, 3472-83	16.4	60
292	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	3.9	60
291	Calculation of origin-independent optical rotation tensor components in approximate time-dependent density functional theory. *Journal of Chemical Physics*, **2006**, 125, 34102	3.9	60
290	Relativistic Density-Functional Computations of the Chemical Shift of 129Xe in . *Journal of Physical Chemistry A*, **2003**, 107, 4967-4972	2.8	59
289	Relativistic Zeroth-Order Regular Approximation Combined with Nonhybrid and Hybrid Density Functional Theory: Performance for NMR Indirect Nuclear Spin-Spin Coupling in Heavy Metal Compounds. *Journal of Chemical Theory and Computation*, **2010**, 6, 223-34	6.4	58
288	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	1.7	57

287	Multifunctional and reactive enantiopure organometallic helicenes: tuning chiroptical properties by structural variations of mono- and bis(platinahelicene)s. *Chemistry - A European Journal*, **2011**, 17, 14178-98	4.8	56
286	A theoretical investigation of the remarkable nuclear spin-spin coupling pattern in [(NC)(5)Pt-Tl(CN)](-). *Journal of the American Chemical Society*, **2001**, 123, 5320-4	16.4	56
285	Iron Alkynyl Helicenes: Redox-Triggered Chiroptical Tuning in the IR and Near-IR Spectral Regions and Suitable for Telecommunications Applications. *Angewandte Chemie - International Edition*, **2016**, 55, 8062-6	16.4	55
284	Relativistic calculations of magnetic resonance parameters: background and some recent developments. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2014**, 372, 20120489	3	55
283	Unravelling the structure of Magnus' pink salt. *Journal of the American Chemical Society*, **2014**, 136, 1333-51	11.4	55
282	Calculation of Verdet constants with time-dependent density functional theory: implementation and results for small molecules. *Journal of Chemical Physics*, **2005**, 122, 074105	3.9	55
281	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
280	Solvent effects and dynamic averaging of 195Pt NMR shielding in cisplatin derivatives. *Inorganic Chemistry*, **2011**, 50, 1723-32	5.1	54
279	Two-Component Relativistic Calculations of Electric-Field Gradients Using Exact Decoupling Methods: Spin-orbit and Picture-Change Effects. *Journal of Chemical Theory and Computation*, **2012**, 8, 4239-48	6.4	53
278	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	1.9	53
277	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		53
276	Combined experimental and computational studies of heterobimetallic Bi-Rh paddlewheel carboxylates as catalysts for metal carbenoid transformations. *Journal of Organic Chemistry*, **2009**, 74, 6564-71	4.2	53
275	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, 4836-46	2.8	53
274	Calculating NMR Chemical Shifts for Paramagnetic Metal Complexes from First-Principles. *Journal of Physical Chemistry Letters*, **2015**, 6, 2183-8	6.4	52
273	Importance of vibronic effects on the circular dichroism spectrum of dimethyloxirane. *Journal of Chemical Physics*, **2005**, 122, 234305	3.9	52
272	Temperature dependence of contact and dipolar NMR chemical shifts in paramagnetic molecules. *Journal of Chemical Physics*, **2015**, 142, 054108	3.9	51
271	Theoretical investigation of paramagnetic NMR shifts in transition metal acetylacetonato complexes: analysis of signs, magnitudes, and the role of the covalency of ligand-metal bonding. *Inorganic Chemistry*, **2012**, 51, 8340-51	5.1	51
270	Atomic contributions from spin-orbit coupling to 29Si NMR chemical shifts in metallasilatrane complexes. *Chemistry - A European Journal*, **2012**, 18, 12803-13	4.8	51

269	Enhancement of IR and VCD intensities due to charge transfer. *Physical Chemistry Chemical Physics*, **2009**, 11, 1526-38	3.6	50
268	Spectral and structural characterization of amidate-bridged platinum-thallium complexes with strong metal-metal bonds. *Inorganic Chemistry*, **2006**, 45, 4526-36	5.1	50
267	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	3.9	50
266	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, 10942-54	3.9	50
265	Periodic trends in indirect nuclear spin-spin coupling tensors: relativistic density functional calculations for interhalogen diatomics. *Journal of the American Chemical Society*, **2002**, 124, 4894-900	16.4	50
264	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, 4336-46	6.4	48
263	Calculation of the vibrationally resolved, circularly polarized luminescence of d-camphorquinone and (S,S)-trans-beta-hydrindanone. *ChemPhysChem*, **2010**, 11, 2409-15	3.2	48
262	Calculation of static and dynamic linear magnetic response in approximate time-dependent density functional theory. *Journal of Chemical Physics*, **2007**, 126, 024101	3.9	48
261	A diuranium carbide cluster stabilized inside a C fullerene cage. *Nature Communications*, **2018**, 9, 2753	17.4	47
260	Computational modeling of polyoxotungstates by relativistic DFT calculations of (183)W NMR chemical shifts. *Chemistry - A European Journal*, **2006**, 12, 8460-71	4.8	47
259	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	3.9	46
258	Time dependent density functional theory modeling of chiroptical properties of small amino acids in solution. *Journal of Physical Chemistry A*, **2006**, 110, 4115-23	2.8	46
257	Single-ion 4f element magnetism: an ab-initio look at Ln(COT)2(-). *Dalton Transactions*, **2015**, 44, 19886-900	4.9	45
256	A quantum chemical approach to the design of chiral negative index materials. *Optics Express*, **2007**, 15, 5730-41	3.3	45
255	A density functional study of the 13C NMR chemical shifts in functionalized single-walled carbon nanotubes. *Journal of the American Chemical Society*, **2007**, 129, 4430-9	16.4	45
254	Solvent effects on 195Pt and 205Tl NMR chemical shifts of the complexes [(NC)5Pt--Tl(CN)n]n- (n=0-3), and [(NC)5Pt--Tl--Pt(CN)5]3- studied by relativistic density functional theory. *Chemistry - A European Journal*, **2004**, 10, 2581-9	4.8	45
253	On the origin of the optical activity in the d-d transition region of tris-bidentate Co(III) and Rh(III) complexes. *Inorganic Chemistry*, **2003**, 42, 8902-10	5.1	45
252	Understanding and Controlling the Emission Brightness and Color of Molecular Cerium Luminophores. *Journal of the American Chemical Society*, **2018**, 140, 4588-4595	16.4	44

251	Density Functional Study of the 13C NMR Chemical Shifts in Single-Walled Carbon Nanotubes with Stone–Wales Defects. *Journal of Physical Chemistry C*, **2008**, 112, 11744-11750	3.8	44
250	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	3.9	43
249	NMR properties of platinum--thallium bonded complexes: analysis of relativistic density functional theory results. *Magnetic Resonance in Chemistry*, **2004**, 42 Spec no, S99-S116	2.1	43
248	Variational versus Perturbational Treatment of Spin-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, 1052-67	6.4	42
247	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	3.9	41
246	Calculation of the Term of Magnetic Circular Dichroism. A Time-Dependent Density Functional Theory Approach. *Journal of Chemical Theory and Computation*, **2007**, 3, 434-47	6.4	41
245	A theoretical study of the NMR spin-spin coupling constants of the complexes [(NC)(5)Pt-Tl(CN)(n)](n-) (n = 0-3) and [(NC)(5)Pt-Tl-Pt(CN)(5)](3-): a lesson on environmental effects. *Journal of the American Chemical Society*, **2003**, 125, 13585-93	16.4	41
244	Theoretical studies of surface enhanced hyper-Raman spectroscopy: the chemical enhancement mechanism. *Journal of Chemical Physics*, **2010**, 133, 054103	3.9	40
243	Electronic structure and circular dichroism of tris(bipyridyl) metal complexes within density functional theory. *Inorganic Chemistry*, **2010**, 49, 1355-62	5.1	40
242	Metallahelicenes: Easily Accessible Helicene Derivatives with Large and Tunable Chiroptical Properties. *Angewandte Chemie*, **2010**, 122, 103-106	3.6	40
241	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, 1902-14	6.4	40
240	Application of magnetically perturbed time-dependent density functional theory to magnetic circular dichroism: calculation of B terms. *Journal of Chemical Physics*, **2008**, 128, 144105	3.9	40
239	The accuracy of hyperfine integrals in relativistic NMR computations based on the zeroth-order regular approximation. *Theoretical Chemistry Accounts*, **2004**, 112, 52-57	1.9	40
238	Modulation of circularly polarized luminescence through excited-state symmetry breaking and interbranched exciton coupling in helical push-pull organic systems. *Chemical Science*, **2020**, 11, 567-576	9.4	40
237	Magnetic resonance properties of actinyl carbonate complexes and plutonyl(VI)-tris-nitrate. *Inorganic Chemistry*, **2014**, 53, 8577-92	5.1	39
236	Transuranic Hybrid Materials: Crystallographic and Computational Metrics of Supramolecular Assembly. *Journal of the American Chemical Society*, **2017**, 139, 10843-10855	16.4	39
235	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, 1051-60	6.4	39
234	Impact of the Kohn-Sham Delocalization Error on the 4f Shell Localization and Population in Lanthanide Complexes. *Journal of Chemical Theory and Computation*, **2016**, 12, 3109-21	6.4	38

233	Ruthenium-Grafted Vinylhelicenes: Chiroptical Properties and Redox Switching. *Chemistry - A European Journal*, **2015**, 21, 17100-15	4.8	38
232	Relativistic Density Functional Calculations of Hyperfine Coupling with Variational versus Perturbational Treatment of Spin-Orbit Coupling. *Journal of Chemical Theory and Computation*, **2013**, 9, 1932-48	6.4	38
231	Scalar Relativistic Computations of Nuclear Magnetic Shielding and g-Shifts with the Zeroth-Order Regular Approximation and Range-Separated Hybrid Density Functionals. *Journal of Chemical Theory and Computation*, **2011**, 7, 3278-92	6.4	38
230	Two-component relativistic density functional method for computing nonsingular complex linear response of molecules based on the zeroth order regular approximation. *Journal of Chemical Physics*, **2009**, 130, 194102	3.9	38
229	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, 11508-21	4.3	37
228	Computational study and molecular orbital analysis of NMR shielding, spin-spin coupling, and electric field gradients of azido platinum complexes. *Journal of the American Chemical Society*, **2012**, 134, 13374-85	16.4	37
227	Assembly of helicene-capped N,P,N,P,N-helicands within Cu(I) helicates: impacting chiroptical properties by ligand-ligand charge transfer. *Angewandte Chemie - International Edition*, **2013**, 52, 1968-72	16.4	37
226	Computation of Optical Rotation using Time□Dependent Density Functional Theory. *Computing Letters*, **2007**, 3, 131-150		37
225	Study of static and dynamic first hyperpolarizabilities using time-dependent density functional quadratic response theory with local contribution and natural bond orbital analysis. *Journal of Chemical Physics*, **2006**, 125, 234101	3.9	37
224	Zero-point corrections and temperature dependence of HD spin-spin coupling constants of heavy metal hydride and dihydrogen complexes calculated by vibrational averaging. *Journal of the American Chemical Society*, **2006**, 128, 10060-72	16.4	37
223	Theoretical investigation of the apparently irregular behavior of pt-pt nuclear spin-spin coupling constants. *Journal of the American Chemical Society*, **2003**, 125, 1028-32	16.4	37
222	Electronic Band Shapes Calculated with Optimally Tuned Range-Separated Hybrid Functionals. *Journal of Chemical Theory and Computation*, **2014**, 10, 4599-608	6.4	36
221	Enantiopure Cycloiridiated Complexes Bearing a Pentahelicenic N-Heterocyclic Carbene and Displaying Long-Lived Circularly Polarized Phosphorescence. *Angewandte Chemie*, **2017**, 129, 8348-8351	3.6	35
220	Giant Faraday Rotation in Mesogenic Organic Molecules. *Chemistry of Materials*, **2013**, 25, 1139-1143	9.6	35
219	Orbitals: Some Fiction and Some Facts. *Journal of Chemical Education*, **2012**, 89, 1032-1040	2.4	35
218	Rhodium(II)-Catalyzed Cross-Coupling of Diazo Compounds. *Angewandte Chemie*, **2011**, 123, 2592-2596	3.6	35
217	Electric Field Gradients Calculated from Two-Component Hybrid Density Functional Theory Including Spin-Orbit Coupling. *Journal of Chemical Theory and Computation*, **2010**, 6, 2669-86	6.4	35
216	Computational modeling of the optical rotation of amino acids: a new look at an old rule for pH dependence of optical rotation. *Journal of the American Chemical Society*, **2008**, 130, 4404-14	16.4	35

215	Temperature dependence of the optical rotation of fenchone calculated by vibrational averaging. *Journal of Physical Chemistry A*, **2006**, 110, 11381-3	2.8	35
214	Modeling of heavy-atom-ligand NMR spin-spin coupling in solution: molecular dynamics study and natural bond orbital analysis of Hg-C coupling constants. *Chemistry - A European Journal*, **2011**, 17, 161-73	4.8	34
213	A pragmatic recipe for the treatment of hindered rotations in the vibrational averaging of molecular properties. *ChemPhysChem*, **2008**, 9, 159-70	3.2	34
212	Calculation of Heavy-Nucleus Chemical Shifts. Relativistic All-Electron Methods **2004**, 227-247		34
211	Giant spin-orbit effects on H and C NMR shifts for uranium(vi) complexes revisited: role of the exchange-correlation response kernel, bonding analyses, and new predictions. *Physical Chemistry Chemical Physics*, **2016**, 18, 30462-30474	3.6	33
210	Helicene-grafted vinyl- and carbene-osmium complexes: an example of acid-base chiroptical switching. *Chemical Communications*, **2014**, 50, 2854-6	5.8	33
209	199Hg Shielding Tensor in Methylmercury Halides: NMR Experiments and ZORA DFT Calculations. *Journal of Physical Chemistry A*, **2002**, 106, 9313-9318	2.8	33
208	Engaging the Terminal: Promoting Halogen Bonding Interactions with Uranyl Oxo Atoms. *Chemistry - A European Journal*, **2017**, 23, 15355-15369	4.8	32
207	Chiroptical properties of carbo[6]helicene derivatives bearing extended π-conjugated cyano substituents. *Chirality*, **2013**, 25, 455-65	2.1	31
206	A theoretical study of the large Hg-Hg spin-spin coupling constants in Hg(2)(2+), Hg(3)(2+), and Hg(2)(2+)-crown ether complexes. *Journal of the American Chemical Society*, **2003**, 125, 4937-42	16.4	31
205	Time dependent density functional theory modeling of specific rotation and optical rotatory dispersion of the aromatic amino acids in solution. *Journal of Physical Chemistry A*, **2006**, 110, 12908-17	2.8	30
204	Circular dichroism spectrum of [Co(en)3]3+ in water: A discrete solvent reaction field study. *International Journal of Quantum Chemistry*, **2006**, 106, 2479-2488	2.1	30
203	Relativistic Calculations of Spin–Spin Coupling Constants of Heavy Nuclei **2004**, 249-264		30
202	The unexpected roles of π and σ orbitals in electron donor and acceptor group effects on the C NMR chemical shifts in substituted benzenes. *Chemical Science*, **2017**, 8, 6570-6576	9.4	29
201	Application of magnetically perturbed time-dependent density functional theory to magnetic circular dichroism. III. Temperature-dependent magnetic circular dichroism induced by spin-orbit coupling. *Journal of Chemical Physics*, **2008**, 129, 104105	3.9	29
200	Ab initio calculation of the C/D ratio of magnetic circular dichroism. *Journal of Chemical Physics*, **2005**, 122, 094112	3.9	29
199	Use of N NMR spectroscopy to probe covalency in a thorium nitride. *Chemical Science*, **2019**, 10, 6431-6436	9.4	28
198	Long-Lived Circularly Polarized Phosphorescence in Helicene-NHC Rhenium(I) Complexes: The Influence of Helicene, Halogen, and Stereochemistry on Emission Properties. *Angewandte Chemie - International Edition*, **2020**, 59, 8394-8400	16.4	28

197	Kohn-Sham calculations of NMR shifts for paramagnetic 3d metal complexes: protocols, delocalization error, and the curious amide proton shifts of a high-spin iron(ii) macrocycle complex. *Physical Chemistry Chemical Physics*, **2016**, 18, 21051-68	3.6	28
196	A density functional study of the 13C NMR chemical shifts in fluorinated single-walled carbon nanotubes. *Journal of Physical Chemistry A*, **2009**, 113, 4117-24	2.8	28
195	Determining the Diameter of Functionalized Single-Walled Carbon Nanotubes with 13C NMR: A Theoretical Study. *Journal of Physical Chemistry C*, **2008**, 112, 9267-9271	3.8	28
194	Mechanistic studies of UV assisted [4 + 2] cycloadditions in synthetic efforts toward vibsanin E. *Journal of the American Chemical Society*, **2007**, 129, 10763-72	16.4	28
193	Temperature dependence of the optical rotation in six bicyclic organic molecules calculated by vibrational averaging. *ChemPhysChem*, **2007**, 8, 605-16	3.2	28
192	Diastereo- and enantioselective synthesis of organometallic bis(helicene)s by a combination of C-H activation and dynamic isomerization. *Chemistry - A European Journal*, **2013**, 19, 16722-8	4.8	27
191	Calculation of optical rotatory dispersion and electronic circular dichroism for tris-bidentate groups 8 and 9 metal complexes, with emphasis on exciton coupling. *Journal of Physical Chemistry A*, **2011**, 115, 2635-49	2.8	27
190	Diuranium(IV) Carbide Cluster UC Stabilized Inside Fullerene Cages. *Journal of the American Chemical Society*, **2019**, 141, 20249-20260	16.4	27
189	Ab Initio Study of Covalency in the Ground versus Core-Excited States and X-ray Absorption Spectra of Actinide Complexes. *Journal of Physical Chemistry Letters*, **2018**, 9, 5583-5591	6.4	27
188	A Nonorthogonal State-Interaction Approach for Matrix Product State Wave Functions. *Journal of Chemical Theory and Computation*, **2016**, 12, 5881-5894	6.4	26
187	Effects from spin-orbit coupling on electron-nucleus hyperfine coupling calculated at the restricted active space level for Kramers doublets. *Journal of Chemical Theory and Computation*, **2015**, 11, 538-49	6.4	26
186	Magnetic properties and electronic structures of Ar3U(IV)L Complexes with Ar = C5(CH3)4H(or C5H5(and L = CH3, NO, and Cl. *Inorganic Chemistry*, **2014**, 53, 13174-87	5.1	26
185	NMR measurements and density functional calculations of the 199Hg-13C spin-spin coupling tensor in methylmercury halides. *Journal of Physical Chemistry A*, **2007**, 111, 5343-8	2.8	26
184	Density-Functional Calculation of the 183W and 17O NMR Chemical Shifts for Large Polyoxotungstates. *European Journal of Inorganic Chemistry*, **2006**, 2006, 1139-1148	2.3	26
183	Static and dynamic second hyperpolarizability calculated by time-dependent density functional cubic response theory with local contribution and natural bond orbital analysis. *Journal of Chemical Physics*, **2007**, 127, 074104	3.9	26
182	Relativistic Effects on NMR Parameters. *Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems*, **2013**, 3, 69-117		25
181	Performance of conventional and range-separated hybrid density functionals in calculations of electronic circular dichroism spectra of transition metal complexes. *Journal of Physical Chemistry A*, **2011**, 115, 14677-86	2.8	25
180	NMR computations for carbon nanotubes from first principles: Present status and future directions. *International Journal of Quantum Chemistry*, **2009**, 109, 3343-3367	2.1	25

179	Paramagnetic effects on the NMR spectra of "diamagnetic" ruthenium(bis-phosphine)(bis-semiquinone) complexes. *Inorganic Chemistry*, **2009**, 48, 5504-11	5.1	25
178	Circular dichroism of trigonal dihedral chromium(III) complexes: a theoretical study based on open-shell time-dependent density functional theory. *Inorganic Chemistry*, **2008**, 47, 11656-68	5.1	25
177	A Solid-State NMR, X-ray Diffraction, and Ab Initio Investigation into the Structures of Novel Tantalum Oxyfluoride Clusters. *Chemistry of Materials*, **2008**, 20, 2205-2217	9.6	25
176	DFT Calculations of the 183W NMR Chemical Shifts in Reduced Polyoxotungstates. *European Journal of Inorganic Chemistry*, **2006**, 2006, 1149-1154	2.3	25
175	Relativistic electron densities in the four-component Dirac representation and in the two-component picture. *Theoretical Chemistry Accounts*, **2000**, 104, 82-88	1.9	25
174	Molecular dynamics computational study of the 199Hg-199Hg NMR spin-spin coupling constants of [Hg-Hg-Hg]2+ in SO2 solution. *Journal of the American Chemical Society*, **2007**, 129, 11093-9	16.4	24
173	Achieving high circularly polarized luminescence with push-pull helicenic systems: from rationalized design to top-emission CP-OLED applications. *Chemical Science*, **2021**, 12, 5522-5533	9.4	24
172	Orbitals for Analyzing Bonding and Magnetism of Heavy-Metal Complexes. *Comments on Inorganic Chemistry*, **2016**, 36, 215-244	3.9	23
171	Relativistic hybrid density functional calculations of indirect nuclear spin□spin coupling tensors □ Comparison with experiment for diatomic alkali metal halides,. *Canadian Journal of Chemistry*, **2009**, 87, 927-941	0.9	23
170	Ligand NMR Chemical Shift Calculations for Paramagnetic Metal Complexes: 5f vs 5f Actinides. *Journal of Chemical Theory and Computation*, **2016**, 12, 5309-5321	6.4	23
169	The halogen effect on the C NMR chemical shift in substituted benzenes. *Physical Chemistry Chemical Physics*, **2018**, 20, 11247-11259	3.6	22
168	Electronic and chiroptical properties of chiral cycloiridiated complexes bearing helicenic NHC ligands. *Chemical Communications*, **2016**, 52, 9243-6	5.8	22
167	NMR J-coupling constants in cisplatin derivatives studied by molecular dynamics and relativistic DFT. *ChemPhysChem*, **2011**, 12, 1448-55	3.2	22
166	A New Reaction for Organoselenium Compounds: Alkyl Transfer from Diorganoselenium(IV) Dibromides to Alkenoic Acids To Give □- and □-Lactones. *Organometallics*, **2009**, 28, 3426-3436	3.8	22
165	Iron Alkynyl Helicenes: Redox-Triggered Chiroptical Tuning in the IR and Near-IR Spectral Regions and Suitable for Telecommunications Applications. *Angewandte Chemie*, **2016**, 128, 8194-8198	3.6	22
164	An investigation of chlorine ligands in transition-metal complexes via □□l solid-state NMR and density functional theory calculations. *Inorganic Chemistry*, **2014**, 53, 9581-97	5.1	21
163	Time-dependent density functional theory applied to ligand-field excitations and their circular dichroism in some transition metal complexes. *Chemical Physics*, **2011**, 391, 92-100	2.3	21
162	Molecular orbital analysis of the inverse halogen dependence of nuclear magnetic shielding in LaX□ X = F, Cl, Br, I. *Magnetic Resonance in Chemistry*, **2010**, 48 Suppl 1, S76-85	2.1	21

161	Spirooxazine-based multifunctional molecular switches with tunable photochromism and nonlinear optical response. *Journal of Materials Chemistry C*, **2013**, 1, 5779	7.1	20
160	Solid-state NMR spectroscopic study of coordination compounds of XeF(2) with metal cations and the crystal structure of [Ba(XeF(2))(5)][AsF(6)](2). *Inorganic Chemistry*, **2007**, 46, 6069-77	5.1	20
159	Density Functional Study of H-D Coupling Constants in Heavy Metal Dihydrogen and Dihydride Complexes: The Role of Geometry, Spin-Orbit Coupling, and Gradient Corrections in the Exchange-Correlation Kernel. *Journal of Chemical Theory and Computation*, **2005**, 1, 601-11	6.4	20
158	Axially and Helically Chiral Cationic Radical Bicarbazoles: SOMO-HOMO Level Inversion and Chirality Impact on the Stability of Mono- and Diradical Cations. *Journal of the American Chemical Society*, **2020**,	16.4	20
157	Large-Scale Synthesis of Helicene-Like Molecules for the Design of Enantiopure Thin Films with Strong Chiroptical Activity. *Chemistry - A European Journal*, **2016**, 22, 3333-3346	4.8	20
156	Low-Spin Fe(III) Macrocyclic Complexes of Imidazole-Appended 1,4,7-Triazacyclononane as Paramagnetic Probes. *Inorganic Chemistry*, **2018**, 57, 8364-8374	5.1	20
155	Redox-Active Chiroptical Switching in Mono- and Bis-Iron Ethynylcarbo[6]helicenes Studied by Electronic and Vibrational Circular Dichroism and Resonance Raman Optical Activity. *Chemistry - A European Journal*, **2018**, 24, 15067-15079	4.8	19
154	Helicenes Grafted with 1,1,4,4-Tetracyanobutadiene Moieties: Helical Push-Pull Systems with Strong Electronic Circular Dichroism and Two-Photon Absorption. *Chemistry - A European Journal*, **2018**, 24, 14484-14494	4.8	19
153	Magnetic circular dichroism of UCl in the ligand-to-metal charge-transfer spectral region. *Physical Chemistry Chemical Physics*, **2017**, 19, 17300-17313	3.6	19
152	Time-dependent density functional methods for surface enhanced Raman scattering (SERS) studies. *Computational and Theoretical Chemistry*, **2012**, 987, 32-41	2	19
151	Quadrupolar NMR Spin Relaxation Calculated Using Ab Initio Molecular Dynamics: Group 1 and Group 17 Ions in Aqueous Solution. *Journal of Chemical Theory and Computation*, **2013**, 9, 4074-86	6.4	19
150	Synthesis and evaluation of tetracycline imprinted xerogels: comparison of experiment and computational modeling. *Analytica Chimica Acta*, **2011**, 684, 63-71	6.6	19
149	Puzzling Lack of Temperature Dependence of the PuO Magnetic Susceptibility Explained According to Ab Initio Wave Function Calculations. *Journal of Physical Chemistry Letters*, **2017**, 8, 673-678	6.4	18
148	Synthesis, Spectroelectrochemical Behavior, and Chiroptical Switching of Tris(diketonato) Complexes of Ruthenium(III), Chromium(III), and Cobalt(III). *Inorganic Chemistry*, **2017**, 56, 4556-4568	5.1	18
147	Homoleptic Aryl Complexes of Uranium (IV). *Angewandte Chemie - International Edition*, **2019**, 58, 10266-10270	16.4	18
146	Iridium(III) Complexes Containing 1,10-Phenanthroline and Derivatives: Synthetic, Stereochemical, and Structural Studies, and their Antimicrobial Activity. *Australian Journal of Chemistry*, **2013**, 66, 1065	1.2	18
145	Electronic to- Excitations of Rhodamine Dyes Exhibit a Time-Dependent Kohn-Sham Theory "Cyanine Problem". *ChemistryOpen*, **2017**, 6, 385-392	2.3	18
144	Electronic Structure and Properties of Berkelium Iodates. *Journal of the American Chemical Society*, **2017**, 139, 13361-13375	16.4	18

143	Simulation of resonance hyper-Rayleigh scattering of molecules and metal clusters using a time-dependent density functional theory approach. *Journal of Chemical Physics*, **2014**, 141, 124305	3.9	18
142	Density functional study of tetraphenylporphyrin long-range exciton coupling. *ChemistryOpen*, **2012**, 1, 184-94	2.3	18
141	Tetracycline speciation during molecular imprinting in xerogels results in class-selective binding. *Analyst, The*, **2011**, 136, 749-55	5	18
140	Density functional computations of 99Ru chemical shifts: relativistic effects, influence of the density functional, and study of solvent effects on fac-[Ru(CO)3I3]-. *Magnetic Resonance in Chemistry*, **2006**, 44, 989-1007	2.1	18
139	Development of a sum-over-states density functional theory for both electric and magnetic static response properties. *Journal of Chemical Physics*, **2007**, 126, 174103	3.9	18
138	Ionic Liquid Solvation versus Catalysis: Computational Insight from a Multisubstituted Imidazole Synthesis in [EtNH][HSO]. *ChemistryOpen*, **2016**, 5, 460-469	2.3	17
137	29Si DFT/NMR Observation of Spin□Orbit Effect in Metallasilatrane Sheds Some Light on the Strength of the Metal-Silicon Interaction. *Angewandte Chemie*, **2011**, 123, 269-273	3.6	17
136	Analyzing molecular static linear response properties with perturbed localized orbitals. *Journal of Chemical Physics*, **2010**, 133, 044109	3.9	17
135	Novel pathways for enhancing nonlinearity of organics utilizing metal clusters. *Journal of Physical Chemistry A*, **2010**, 114, 7590-4	2.8	17
134	Thermochromic Uranyl Isothiocyanates: Influencing Charge Transfer Bands with Supramolecular Structure. *Inorganic Chemistry*, **2018**, 57, 2455-2471	5.1	16
133	Calculation of linear and nonlinear optical properties of azobenzene derivatives with Kohn-Sham and coupled-cluster methods. *Physical Chemistry Chemical Physics*, **2018**, 20, 7303-7316	3.6	16
132	Simulating Third-Order Nonlinear Optical Properties Using Damped Cubic Response Theory within Time-Dependent Density Functional Theory. *Journal of Chemical Theory and Computation*, **2016**, 12, 1294-304	5.4	16
131	Analysis of Proton NMR in Hydrogen Bonds in Terms of Lone-Pair and Bond Orbital Contributions. *Chemistry - A European Journal*, **2015**, 21, 18138-55	4.8	16
130	Assembly of Helicene-Capped N,P,N,P,N-Helicands within CuI Helicates: Impacting Chiroptical Properties by Ligand□Ligand Charge Transfer. *Angewandte Chemie*, **2013**, 125, 2022-2026	3.6	16
129	Fast generation of nonresonant and resonant optical rotatory dispersion curves with the help of circular dichroism calculations and Kramers-Kronig transformations. *Chirality*, **2008**, 20, 995-1008	2.1	16
128	Where Do the Forces in Molecules Come from? A Density Functional Study of N2 and HCl. *Journal of Physical Chemistry A*, **2000**, 104, 6039-6046	2.8	16
127	Computational prediction and analysis of the (27)Al solid-state NMR spectrum of methylaluminoxane (MAO) at variable temperatures and field strengths. *Physical Chemistry Chemical Physics*, **2016**, 18, 24106-18	3.6	15
126	X-ray circular dichroism signals: a unique probe of local molecular chirality. *Chemical Science*, **2017**, 8, 5969-5978	9.4	15

125	NMR Calculations for Paramagnetic Molecules and Metal Complexes. *Annual Reports in Computational Chemistry*, **2015**, 11, 3-36	1.8	15
124	AB Initio Electronic Circular Dichroism and Optical Rotatory Dispersion: From Organic Molecules to Transition Metal Complexes **2012**, 593-642		15
123	13C 77Se and 77Se 77Se spin spin coupling tensors in carbon diselenide: NMR experiments and ZORA DFT calculations. *Physical Chemistry Chemical Physics*, **2003**, 5, 4551-4555	3.6	15
122	Relativistic Effects on Magnetic Resonance Parameters and Other Properties of Inorganic Molecules and Metal Complexes. *Challenges and Advances in Computational Chemistry and Physics*, **2010**, 521-598	0.7	15
121	Synthesis, Characterization, and Electrochemistry of the Homoleptic f Element Ketimide Complexes [Li][M(N?CBuPh)] (M = Ce, Th). *Inorganic Chemistry*, **2019**, 58, 12654-12661	5.1	14
120	Ab Initio Study of Circular Dichroism and Circularly Polarized Luminescence of Spin-Allowed and Spin-Forbidden Transitions: From Organic Ketones to Lanthanide Complexes. *Journal of Chemical Theory and Computation*, **2019**, 15, 4140-4155	6.4	14
119	Effects of stereoelectronic interactions on the relativistic spin-orbit and paramagnetic components of the (13)C NMR shielding tensors of dihaloethenes. *Physical Chemistry Chemical Physics*, **2015**, 17, 19315-24	3.6	14
118	Reactions of gold(III) complexes with alkenes in aqueous media: generation of bis-(hydroxyalkyl)gold(III) complexes. *Journal of Coordination Chemistry*, **2013**, 66, 1153-1165	1.6	14
117	Microscopic cascading of second-order molecular nonlinearity: New design principles for enhancing third-order nonlinearity. *Optics Express*, **2010**, 18, 8713-21	3.3	14
116	A gauge-origin independent expression for the Verdet constant within the time-dependent density functional theory. *International Journal of Quantum Chemistry*, **2005**, 101, 572-578	2.1	14
115	Ab Initio Analysis of Metal-Ligand Bonding in An(COT) with An=Th, U in Their Ground- and Core-Excited States. *Chemistry - A European Journal*, **2020**, 26, 1776-1788	4.8	14
114	Bimetallic Gold(I) Complexes with Ethynyl-Helicene and Bis-Phosphole Ligands: Understanding the Role of Aurophilic Interactions in their Chiroptical Properties. *Chemistry - A European Journal*, **2016**, 22, 6075-86	4.8	14
113	Calculated Resonance Vibrational Raman Optical Activity Spectra of Naproxen and Ibuprofen. *Journal of Physical Chemistry A*, **2016**, 120, 9740-9748	2.8	14
112	Nuclear Magnetic Resonance Measurements and Electronic Structure of Pu(IV) in [(Me)4N]2PuCl6. *Inorganic Chemistry*, **2016**, 55, 8371-80	5.1	14
111	Magnetic circular dichroism spectra of transition metal complexes calculated from restricted active space wavefunctions. *Physical Chemistry Chemical Physics*, **2019**, 21, 5586-5597	3.6	14
110	Structure and Bonding Investigation of Plutonium Peroxocarbonate Complexes Using Cerium Surrogates and Electronic Structure Modeling. *Inorganic Chemistry*, **2017**, 56, 791-801	5.1	13
109	Crystal Field in Rare-Earth Complexes: From Electrostatics to Bonding. *Chemistry - A European Journal*, **2018**, 24, 5538-5550	4.8	13
108	Assessment of Tuned Range Separated Exchange Functionals for Spectroscopies and Properties of Uranium Complexes. *Journal of Chemical Theory and Computation*, **2017**, 13, 3614-3625	6.4	13

107	Experimental and theoretical investigations of selenium nuclear magnetic shielding tensors in Se□N heterocycles. *Canadian Journal of Chemistry*, **2009**, 87, 1546-1564	0.9	13
106	Why the Particle-in-a-Box Model Works Well for Cyanine Dyes but Not for Conjugated Polyenes. *Journal of Chemical Education*, **2007**, 84, 1840	2.4	13
105	Compression of curium pyrrolidine-dithiocarbamate enhances covalency. *Nature*, **2020**, 583, 396-399	50.4	13
104	Palladium Acetate Revisited: Unusual Ring-Current Effects, One-Electron Reduction, and Metal-Metal Bonding. *Inorganic Chemistry*, **2018**, 57, 8046-8049	5.1	13
103	Relativistic Effects on Electron-Nucleus Hyperfine Coupling Studied with an Exact 2-Component (X2C) Hamiltonian. *Journal of Chemical Theory and Computation*, **2017**, 13, 710-718	6.4	12
102	Probing the Electronic Structure of a Thorium Nitride Complex by Solid-State N NMR Spectroscopy. *Inorganic Chemistry*, **2020**, 59, 10138-10145	5.1	12
101	Similar ligand-metal bonding for transition metals and actinides? 5f U(CH) 3d metallocenes. *Chemical Science*, **2018**, 9, 6292-6306	9.4	12
100	Computation of Chemical Shifts for Paramagnetic Molecules: A Laboratory Experiment for the Undergraduate Curriculum. *Journal of Chemical Education*, **2014**, 91, 1058-1063	2.4	12
99	Computational Modeling of the Optical Rotation of Amino Acids: An □n Silico□Experiment for Physical Chemistry. *Journal of Chemical Education*, **2013**, 90, 656-660	2.4	12
98	Synthesis and characterization of the trihalophosphine compounds of ruthenium [RuX2(eta(6)-cymene)(PY3)] (X = Cl, Br, Y = F, Cl, Br) and the related PF2(NMe2) and P(NMe2)3 compounds; multinuclear NMR spectroscopy and the X-ray single crystal structures of [RuBr2(eta(6)-cymene)(PF3)], [RuBr2(eta(6)-cymene)(PF2{NMe2})], and	5.1	12
97	The "invisible" 13C NMR chemical shift of the central carbon atom in [(Ph3PAu)6C]2+: a theoretical investigation. *Chemistry - A European Journal*, **2005**, 11, 1677-86	4.8	12
96	Uranyl Carbonate Complexes in Aqueous Solution and Their Ligand NMR Chemical Shifts and O Quadrupolar Relaxation Studied by ab Initio Molecular Dynamics. *Inorganic Chemistry*, **2017**, 56, 7384-7396	5.1	11
95	Derivation of the RPA (Random Phase Approximation) Equation of ATDDFT (Adiabatic Time Dependent Density Functional Ground State Response Theory) from an Excited State Variational Approach Based on the Ground State Functional. *Journal of Chemical Theory and Computation*, **2014**, 10, 3980-6	6.4	11
94	Experimental and theoretical investigations of the thermodynamic stability of Ba-c(60) and K-C(60) compound clusters. *ACS Nano*, **2008**, 2, 1000-14	16.7	11
93	Quadrupolar N NMR Relaxation from Force-Field and Ab Initio Molecular Dynamics in Different Solvents. *Journal of Chemical Theory and Computation*, **2019**, 15, 509-519	6.4	11
92	Extended H□kel Calculations on Solids Using the Avogadro Molecular Editor and Visualizer. *Journal of Chemical Education*, **2018**, 95, 331-337	2.4	11
91	Experimental and computational study of metal-free Br□sted acidic ionic liquid catalyzed benzylic C(sp3) H bond activation and C N, C C cross couplings. *Journal of Molecular Liquids*, **2019**, 280, 410-419	6	10
90	Long-Lived Circularly Polarized Phosphorescence in Helicene-NHC Rhenium(I) Complexes: The Influence of Helicene, Halogen, and Stereochemistry on Emission Properties. *Angewandte Chemie*, **2020**, 132, 8472-8478	3.6	10

89	Calculation of Dipole-Forbidden 5f Absorption Spectra of Uranium(V) Hexa-Halide Complexes. *Journal of Physical Chemistry Letters*, **2018**, 9, 887-894	6.4	10
88	Calculating Electronic Optical Activity of Coordination Compounds **2013**, 407-426		10
87	Quadrupolar NMR Relaxation from ab Initio Molecular Dynamics: Improved Sampling and Cluster Models versus Periodic Calculations. *Journal of Chemical Theory and Computation*, **2017**, 13, 4397-4409	6.4	10
86	Toward a generalization of the Clough-Lutz-Jirgensons effect: Chiral organic acids with alkyl, hydroxyl, and halogen substituents. *Chirality*, **2010**, 22 Suppl 1, E81-95	2.1	10
85	Time-dependent density-functional-theory calculation of the van der Waals coefficient C6 of alkali-metal atoms Li, Na, K; alkali-metal dimers Li2, Na2, K2; sodium clusters Nan; and fullerene C60. *Physical Review A*, **2008**, 78,	2.6	10
84	Vibrational corrections to magneto-optical rotation: a computational study. *Journal of Physical Chemistry A*, **2007**, 111, 5563-71	2.8	10
83	Magic alkali-fullerene compound clusters of extreme thermal stability. *Journal of Chemical Physics*, **2006**, 125, 191102	3.9	10
82	Redox-triggered chiroptical switching activity of ruthenium(III)-bis-(□diketonato) complexes bearing a bipyridine-helicene ligand. *Chirality*, **2018**, 30, 592-601	2.1	10
81	Influence of Substituents on the Electronic Structure of Mono- and Bis(phosphido) Thorium(IV) Complexes. *Inorganic Chemistry*, **2018**, 57, 7270-7278	5.1	10
80	NMR J-Coupling Constants of Tl-Pt Bonded Metal Complexes in Aqueous Solution: Ab Initio Molecular Dynamics and Localized Orbital Analysis. *Inorganic Chemistry*, **2016**, 55, 12011-12023	5.1	9
79	Insight into the Electronic Structure of Formal Lanthanide(II) Complexes using Magnetic Circular Dichroism Spectroscopy. *Organometallics*, **2019**, 38, 3124-3131	3.8	9
78	Computational analysis of (47/49)Ti NMR shifts and electric field gradient tensors of half-titanocene complexes: structure-bonding-property relationships. *Chemistry - A European Journal*, **2013**, 19, 12018-33	4.8	9
77	Relativistic Theories of NMR Shielding **2017**, 657-692		9
76	[Pt@Pb12]2□A challenging system for relativistic density functional theory calculations of 195Pt and 207Pb NMR parameters. *Canadian Journal of Chemistry*, **2011**, 89, 814-821	0.9	9
75	NMR spin-spin coupling constants: bond angle dependence of the sign and magnitude of the vicinal (3)JHF coupling. *Physical Chemistry Chemical Physics*, **2016**, 18, 24119-28	3.6	9
74	Molecular QTAIM Topology Is Sensitive to Relativistic Corrections. *Chemistry - A European Journal*, **2019**, 25, 2538-2544	4.8	9
73	A Pseudotetrahedral Uranium(V) Complex. *Inorganic Chemistry*, **2018**, 57, 8106-8115	5.1	9
72	Size evolution relativistic DFT-QTAIM study on the gold cluster complexes Au4-S-CnH2n-S?-Au4? (n = 2□). *Chemical Physics Letters*, **2016**, 660, 287-294	2.5	8

71	Calculation of nuclear spin-spin coupling constants using frozen density embedding. *Journal of Chemical Physics*, **2014**, 140, 104107	3.9	8
70	Determination of the structures of molecularly imprinted polymers and xerogels using an automated stochastic approach. *Analytical Chemistry*, **2013**, 85, 8577-84	7.8	8
69	Relativistic Methods for Calculating Electron Paramagnetic Resonance (EPR) Parameters **2017**, 725-763		8
68	Synthesis and Characterization of Two Uranyl-Aryl "Ate" Complexes. *Chemistry - A European Journal* , **2021**, 27, 5885-5889	4.8	8
67	New class of cocogem surfactants based on hexamethylenediamine, propylene oxide, and long chain carboxylic acids: Theory and application. *Journal of Industrial and Engineering Chemistry*, **2020**, 86, 123-135	6.3	7
66	Size evolution study of "molecular" and "atom-in-cluster" polarizabilities of medium-size gold clusters. *Journal of Chemical Physics*, **2011**, 135, 034109	3.9	7
65	Ligand effects on electronic structure and bonding in U(III) coordination complexes: a combined MCD, EPR and computational study. *Dalton Transactions*, **2020**, 49, 14401-14410	4.3	7
64	Isolation and characterization of a covalent Ce-Aryl complex with an anomalous C chemical shift. *Nature Communications*, **2021**, 12, 1713	17.4	7
63	Probing Multiconfigurational States by Spectroscopy: The Cerium XAS L -edge Puzzle. *Chemistry - A European Journal*, **2021**, 27, 7239-7251	4.8	7
62	Why is the Energy of the Singly Occupied Orbital in Some Radicals below the Highest Occupied Orbital Energy?. *Chemistry of Materials*, **2021**, 33, 3678-3691	9.6	7
61	Magnetic Coupling in the Ce(III) Dimer Ce(COT). *Inorganic Chemistry*, **2019**, 58, 581-593	5.1	7
60	Aggregation and antimicrobial properties of gemini surfactants with mono- and di-(2-hydroxypropyl)ammonium head-groups: Effect of the spacer length and computational studies. *Journal of Molecular Liquids*, **2020**, 302, 112579	6	6
59	The Computational Design of Two-Dimensional Materials. *Journal of Chemical Education*, **2019**, 96, 2308-2314	2.4	6
58	Optically active tetra-tert-butyl-P(5)-deltacyclene epimers: preparation, spectroscopy, dynamic equilibriums, H/D exchange, and transition-metal complex chemistry. *Chemistry - A European Journal*, **2014**, 20, 5708-20	4.8	6
57	A new Pu(iii) coordination geometry in (CHNBr)[PuCl(HO)]□2Cl□2HO as obtained via supramolecular assembly in aqueous, high chloride media. *Chemical Communications*, **2017**, 53, 10816-10819	5.8	6
56	Complete Active Space Wavefunction-Based Analysis of Magnetization and Electronic Structure. *Topics in Organometallic Chemistry*, **2018**, 355-390	0.6	6
55	Electron-Nucleus Hyperfine Coupling Calculated from Restricted Active Space Wavefunctions and an Exact Two-Component Hamiltonian. *Journal of Chemical Theory and Computation*, **2021**, 17, 255-268	6.4	6
54	Computational investigation of catalytic effects of CXCOOH (X = F,Cl,H) on the three-component cyclocondensation reaction. *Journal of Molecular Modeling*, **2019**, 25, 173	2	5

53	The Exceptional Diversity of Homoleptic Uranium-Methyl Complexes. *Angewandte Chemie - International Edition*, **2020**, 59, 13586-13590	16.4	5
52	Unveiling the catalytic effects of Br□sted acidic ionic liquid on quantitative □-glucose conversion to 5-HMF: Experimental and computational studies. *Renewable Energy*, **2021**, 171, 383-390	8.1	5
51	Ab Initio Study of Vibronic and Magnetic 5f-to-5f and Dipole-Allowed 5f-to-6d and Charge-Transfer Transitions in [UX] (X = Cl, Br; = 1, 2). *Journal of Chemical Theory and Computation*, **2020**, 16, 5189-5202	6.4	4
50	The Sodium Anion Is Strongly Perturbed in the Condensed Phase Even Though It Appears Like a Free Ion in Nuclear Magnetic Resonance Experiments. *Journal of Physical Chemistry Letters*, **2020**, 11, 843-850	6.4	4
49	Homoleptic Aryl Complexes of Uranium (IV). *Angewandte Chemie*, **2019**, 131, 10372-10376	3.6	4
48	Quadrupolar NMR Relaxation of Aqueous I, Xe, and Cs: A First-Principles Approach from Dynamics to Properties. *Journal of Chemical Theory and Computation*, **2020**, 16, 5835-5844	6.4	4
47	Dinuclear Rhenium Complexes with a Bridging Helicene-bis-bipyridine Ligand: Synthesis, Structure, and Photophysical and Chiroptical Properties. *ChemPlusChem*, **2020**, 85, 2446-2454	2.8	4
46	Validation of microscopic magnetochiral dichroism theory. *Science Advances*, **2021**, 7,	14.3	4
45	UCN@(6)-C: An Encapsulated Triangular UCN Cluster with Ambiguous U Oxidation State [U(III) versus U(I)]. *Journal of the American Chemical Society*, **2021**, 143, 16226-16234	16.4	4
44	Synthesis of Parent Acetylide and Dicarbide Complexes of Thorium and Uranium and an Examination of Their Electronic Structures. *Inorganic Chemistry*, **2021**, 60, 15413-15420	5.1	4
43	Construction of New Azo-group Containing Polycyclic Imidazole Derivatives: Computational Mechanistic, Structural, and Fluorescence Studies. *ChemistrySelect*, **2020**, 5, 6224-6229	1.8	3
42	Gas-Phase Complexes of Americium and Lanthanides with a Bis-triazinyl Pyridine: Reactivity and Bonding of Archetypes for F-Element Separations. *Journal of Physical Chemistry A*, **2020**, 124, 2982-2990	2.8	3
41	Theoretical study of the Raman optical activity spectra of with M□□Co, Rh. *Chirality*, **2020**, 32, 741-752	2.1	3
40	Molecular (global) and atom-in-cluster (local) polarizabilities of medium-size gold nanoclusters: isomer structure effects. *European Physical Journal D*, **2013**, 67, 1	1.3	3
39	Calculating NMR Chemical Shifts and J-Couplings for Heavy Element Compounds **2014**, 1-14		3
38	Covalency in actinide(iv) hexachlorides in relation to the chlorine K-edge X-ray absorption structure.. *Chemical Science*, **2022**, 13, 3194-3207	9.4	3
37	Covalency of Trivalent Actinide Ions with Different Donor Ligands: Do Density Functional and Multiconfigurational Wavefunction Calculations Corroborate the Observed "Breaks"?. *Inorganic Chemistry*, **2021**, 60, 17744-17757	5.1	3
36	Counterion-coupled gemini surfactants based on propoxylated hexamethylenediamine and fatty acids: Theory and application. *Journal of Molecular Liquids*, **2020**, 318, 114050	6	3

35	Proton NMR relaxation from molecular dynamics: intramolecular and intermolecular contributions in water and acetonitrile. *Physical Chemistry Chemical Physics*, **2019**, 21, 26621-26629	3.6	3
34	Axial and helical thermally activated delayed fluorescence bicarbazole emitters: opposite modulation of circularly polarized luminescence through intramolecular charge-transfer dynamics. *Journal of Materials Chemistry C*, **2021**, 9, 11905-11914	7.1	3
33	Valence-shell photoelectron circular dichroism of ruthenium(III)-tris-(acetylacetonato) gas-phase enantiomers. *Physical Chemistry Chemical Physics*, **2021**, 23, 24140-24153	3.6	3
32	molecular dynamics study of sodium NMR chemical shifts in the methylamine solution of [Na [2.2.2]cryptand Na]. *Physical Chemistry Chemical Physics*, **2021**, 23, 339-346	3.6	3
31	Exciton coupling chirality in helicene-porphyrin conjugates. *Chemical Communications*, **2021**, 57, 10743-10746	5.8	3
30	Plutonium chlorido nitrato complexes: ligand competition and computational metrics for assembly and bonding. *Chemical Communications*, **2018**, 54, 12014-12017	5.8	3
29	Homoleptic Perchlorophenyl "Ate" Complexes of Thorium(IV) and Uranium(IV). *Inorganic Chemistry*, **2021**, 60, 12436-12444	5.1	3
28	Computational Tools for Predictive Modeling of Properties in Complex Actinide Systems **2015**, 299-342		2
27	Relativistic Methods for Calculating Electron Paramagnetic Resonance (EPR) Parameters **2015**, 1-39		2
26	Assessment of the Performance of Optimally Tuned Range-Separated Hybrid Functionals for Nuclear Magnetic Shielding Calculations. *Advanced Theory and Simulations*, **2020**, 3, 2000083	3.5	2
25	Size evolution study on the electronic and optical properties of gold-cluster complexes Au4-S-CnH2n-S?-Au4? (n = 2). *Chemical Physics Letters*, **2019**, 732, 136625	2.5	2
24	Relativistic Computation of NMR Shieldings and Spin-Spin Coupling Constants **2007**,		2
23	Spin-Orbit Natural Transition Orbitals and Spin-Forbidden Transitions. *Journal of Chemical Theory and Computation*, **2021**,	6.4	2
22	Luminescent Chiral Exciplexes with Sky-Blue and Green Circularly Polarized-Thermally Activated Delayed Fluorescence. *Chemistry - A European Journal*, **2021**, 27, 16505-16511	4.8	2
21	Relativistic Theories of NMR Shielding **2015**, 1-33		2
20	Cerium(iv) complexes with guanidinate ligands: intense colors and anomalous electronic structures. *Chemical Science*, **2020**, 12, 3558-3567	9.4	2
19	Backbonding in Thorium(IV) and Uranium(IV) Diarsenido Complexes with tBuNC and CO. *Chemistry - A European Journal*, **2021**, 27, 14396-14400	4.8	2
18	Spectroscopic characterization of neptunium(VI), plutonium(VI), americium(VI) and neptunium(V) encapsulated in uranyl nitrate hexahydrate. *Physical Chemistry Chemical Physics*, **2021**, 23, 13228-13241	3.6	2

17	Spectroscopic Properties Obtained from Time-Dependent Density Functional Theory (TD-DFT) **2009**,		1
16	Density Functional Studies of the 13C NMR Chemical Shifts in Single-Walled Carbon Nanotubes. *AIP Conference Proceedings*, **2007**,	0	1
15	Downfolding and N-ization of Basis Sets of Slater Type Orbitals. *AIP Conference Proceedings*, **2007**,	0	1
14	Synthesis and electronic structure analysis of the actinide allenylidenes, [{(NR)}An(CCCPh)] (An = U, Th; R = SiMe). *Chemical Science*, **2021**, 12, 14383-14388	9.4	1
13	The Exceptional Diversity of Homoleptic Uranium-Methyl Complexes. *Angewandte Chemie*, **2020**, 132, 13688-13692	3.6	1
12	Probing Multiconfigurational States by Spectroscopy: The Cerium XAS L -edge Puzzle. *Chemistry - A European Journal*, **2021**, 27, 7188	4.8	1
11	Synthesis and Properties of Partially Saturated Fluorenyl-Derived [n]Helicenes Featuring an Overcrowded Alkene. *Chemistry - A European Journal*, **2021**, 27, 7722-7730	4.8	1
10	Solvent effect on the Pt NMR properties in pyridonate-bridged Pt dinuclear complex derivatives investigated by ab initio molecular dynamics and localized orbital analysis. *Physical Chemistry Chemical Physics*, **2021**, 23, 12864-12880	3.6	1
9	Theoretical Prediction and Interpretation of Np Mössbauer Isomer Shifts. *Journal of Chemical Theory and Computation*, **2021**, 17, 6166-6179	6.4	1
8	Enhanced 5f-δ bonding in [U(CH)]: C K-edge XAS, magnetism, and calculations. *Chemical Communications*, **2021**, 57, 9562-9565	5.8	1
7	Near-infrared -term MCD spectroscopy of octahedral uranium(V) complexes. *Dalton Transactions*, **2021**, 50, 5483-5492	4.3	1
6	Comparative Study of Vibrational Raman Optical Activity with Different Time-Dependent Density Functional Approximations: The VROA36 Database.. *Journal of Physical Chemistry A*, **2022**, 126, 2909-2927	2.8	1
5	Optical Activity of Spin-Forbidden Electronic Transitions in Metal Complexes from Time-Dependent Density Functional Theory with Spin-Orbit Coupling.. *ChemistryOpen*, **2022**, 11, e202200020	2.3	1
4	Phosphahelicenes with (Thio)Phosphinic Acid and Ester Functions by the Oxidative Photocyclisation Approach. *Chemistry - A European Journal*, **2019**, 25, 15609-15614	4.8	0
3	Calculating the Raman and HyperRaman Spectra of Large Molecules and Molecules Interacting with Nanoparticles **2011**, 493-514		
2	Computational mechanistic studies of the carbon-carbon double bond difunctionalization via epoxidation and subsequent aminolysis in vegetable oils. *International Journal of Quantum Chemistry*, **2021**, 121, e26609	2.1	
1	Electronic Structure of the Actinide Elements **2018**, 1-16		