Jochen Autschbach

List of Publications by Year in Descending Order

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	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
375	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
374	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
373	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
372	Spin-Orbit Natural Transition Orbitals and Spin-Forbidden Transitions. *Journal of Chemical Theory and Computation*, **2021**,	6.4	2
371	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
370	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
369	Isolation and characterization of a covalent Ce-Aryl complex with an anomalous C chemical shift. *Nature Communications*, **2021**, 12, 1713	17.4	7
368	Probing Multiconfigurational States by Spectroscopy: The Cerium XAS L -edge Puzzle. *Chemistry - A European Journal*, **2021**, 27, 7239-7251	4.8	7
367	Probing Multiconfigurational States by Spectroscopy: The Cerium XAS L -edge Puzzle. *Chemistry - A European Journal*, **2021**, 27, 7188	4.8	1
366	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
365	Validation of microscopic magnetochiral dichroism theory. *Science Advances*, **2021**, 7,	14.3	4
364	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
363	Unveiling the catalytic effects of Brønsted acidic ionic liquid on quantitative β-glucose conversion to 5-HMF: Experimental and computational studies. *Renewable Energy*, **2021**, 171, 383-390	8.1	5
362	Synthesis and Characterization of Two Uranyl-Aryl "Ate" Complexes. *Chemistry - A European Journal* , **2021**, 27, 5885-5889	4.8	8
361	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
360	Valence-shell photoelectron circular dichroism of ruthenium(III)-tris-(acetylacetonato) gas-phase enantiomers. *Physical Chemistry Chemical Physics*, **2021**, 23, 24140-24153	3.6	3

359	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
358	Exciton coupling chirality in helicene-porphyrin conjugates. *Chemical Communications*, **2021**, 57, 10743-10746	4.2	3
357	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
356	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	
355	Homoleptic Perchlorophenyl "Ate" Complexes of Thorium(IV) and Uranium(IV). *Inorganic Chemistry*, **2021**, 60, 12436-12444	5.1	3
354	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
353	Backbonding in Thorium(IV) and Uranium(IV) Diarsenido Complexes with tBuNC and CO. *Chemistry - A European Journal*, **2021**, 27, 14396-14400	4.8	2
352	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
351	Theoretical Prediction and Interpretation of Np M□ssbauer Isomer Shifts. *Journal of Chemical Theory and Computation*, **2021**, 17, 6166-6179	6.4	1
350	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
349	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
348	Enhanced 5f-□bonding in [U(CH)]: C K-edge XAS, magnetism, and calculations. *Chemical Communications*, **2021**, 57, 9562-9565	5.8	1
347	Near-infrared -term MCD spectroscopy of octahedral uranium(V) complexes. *Dalton Transactions*, **2021**, 50, 5483-5492	4.3	1
346	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
345	The Exceptional Diversity of Homoleptic Uranium-Methyl Complexes. *Angewandte Chemie - International Edition*, **2020**, 59, 13586-13590	16.4	5
344	Construction of New Azo-group Containing Polycyclic Imidazole Derivatives: Computational Mechanistic, Structural, and Fluorescence Studies. *ChemistrySelect*, **2020**, 5, 6224-6229	1.8	3
343	NWChem: Past, present, and future. *Journal of Chemical Physics*, **2020**, 152, 184102	3.9	187
342	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

341	Modern quantum chemistry with [Open]Molcas. *Journal of Chemical Physics*, **2020**, 152, 214117	3.9	106
340	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
339	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
338	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
337	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
336	Theoretical study of the Raman optical activity spectra of with M□□Co, Rh. *Chirality*, **2020**, 32, 741-752	2.1	3
335	Probing the Electronic Structure of a Thorium Nitride Complex by Solid-State N NMR Spectroscopy. *Inorganic Chemistry*, **2020**, 59, 10138-10145	5.1	12
334	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
333	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
332	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
331	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
330	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
329	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
328	Compression of curium pyrrolidine-dithiocarbamate enhances covalency. *Nature*, **2020**, 583, 396-399	50.4	13
327	The Exceptional Diversity of Homoleptic Uranium□Methyl Complexes. *Angewandte Chemie*, **2020**, 132, 13688-13692	3.6	1
326	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
325	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
324	Counterion-coupled gemini surfactants based on propoxylated hexamethylenediamine and fatty acids: Theory and application. *Journal of Molecular Liquids*, **2020**, 318, 114050	6	3

323	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
322	Cerium(iv) complexes with guanidinate ligands: intense colors and anomalous electronic structures. *Chemical Science*, **2020**, 12, 3558-3567	9.4	2
321	OpenMolcas: From Source Code to Insight. *Journal of Chemical Theory and Computation*, **2019**, 15, 5925-5964	5.4	310
320	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
319	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
318	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
317	Use of N NMR spectroscopy to probe covalency in a thorium nitride. *Chemical Science*, **2019**, 10, 6431-6436	9.4	28
316	Homoleptic Aryl Complexes of Uranium (IV). *Angewandte Chemie - International Edition*, **2019**, 58, 10266-10270	16.4	18
315	Experimental and computational study of metal-free Brønsted 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
314	The Computational Design of Two-Dimensional Materials. *Journal of Chemical Education*, **2019**, 96, 2308-2314	2.4	6
313	Insight into the Electronic Structure of Formal Lanthanide(II) Complexes using Magnetic Circular Dichroism Spectroscopy. *Organometallics*, **2019**, 38, 3124-3131	3.8	9
312	Homoleptic Aryl Complexes of Uranium (IV). *Angewandte Chemie*, **2019**, 131, 10372-10376	3.6	4
311	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
310	Phosphahelicenes with (Thio)Phosphinic Acid and Ester Functions by the Oxidative Photocyclisation Approach. *Chemistry - A European Journal*, **2019**, 25, 15609-15614	4.8	0
309	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
308	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
307	Diuranium(IV) Carbide Cluster UC Stabilized Inside Fullerene Cages. *Journal of the American Chemical Society*, **2019**, 141, 20249-20260	16.4	27
306	Magnetic Coupling in the Ce(III) Dimer Ce(COT). *Inorganic Chemistry*, **2019**, 58, 581-593	5.1	7

305	Molecular QTAIM Topology Is Sensitive to Relativistic Corrections. *Chemistry - A European Journal*, **2019**, 25, 2538-2544	4.8	9
304	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
303	Thermochromic Uranyl Isothiocyanates: Influencing Charge Transfer Bands with Supramolecular Structure. *Inorganic Chemistry*, **2018**, 57, 2455-2471	5.1	16
302	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
301	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
300	Crystal Field in Rare-Earth Complexes: From Electrostatics to Bonding. *Chemistry - A European Journal*, **2018**, 24, 5538-5550	4.8	13
299	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
298	The halogen effect on the C NMR chemical shift in substituted benzenes. *Physical Chemistry Chemical Physics*, **2018**, 20, 11247-11259	3.6	22
297	A diuranium carbide cluster stabilized inside a C fullerene cage. *Nature Communications*, **2018**, 9, 2753	17.4	47
296	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
295	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
294	Similar ligand-metal bonding for transition metals and actinides? 5f U(CH) 3d metallocenes. *Chemical Science*, **2018**, 9, 6292-6306	9.4	12
293	Extended Hückel Calculations on Solids Using the Avogadro Molecular Editor and Visualizer. *Journal of Chemical Education*, **2018**, 95, 331-337	2.4	11
292	Exciton coupling in diketopyrrolopyrrole-helicene derivatives leads to red and near-infrared circularly polarized luminescence. *Chemical Science*, **2018**, 9, 735-742	9.4	82
291	Electronic Structure of the Actinide Elements **2018**, 1-16		
290	Plutonium chlorido nitrato complexes: ligand competition and computational metrics for assembly and bonding. *Chemical Communications*, **2018**, 54, 12014-12017	5.8	3
289	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
288	Complete Active Space Wavefunction-Based Analysis of Magnetization and Electronic Structure. *Topics in Organometallic Chemistry*, **2018**, 355-390	0.6	6

287	Redox-triggered chiroptical switching activity of ruthenium(III)-bis-(diketonato) complexes bearing a bipyridine-helicene ligand. *Chirality*, **2018**, 30, 592-601	2.1	10
286	Influence of Substituents on the Electronic Structure of Mono- and Bis(phosphido) Thorium(IV) Complexes. *Inorganic Chemistry*, **2018**, 57, 7270-7278	5.1	10
285	A Pseudotetrahedral Uranium(V) Complex. *Inorganic Chemistry*, **2018**, 57, 8106-8115	5.1	9
284	Palladium Acetate Revisited: Unusual Ring-Current Effects, One-Electron Reduction, and Metal-Metal Bonding. *Inorganic Chemistry*, **2018**, 57, 8046-8049	5.1	13
283	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
282	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
281	Calculating Natural Optical Activity of Molecules from First Principles. *Annual Review of Physical Chemistry*, **2017**, 68, 399-420	15.7	88
280	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
279	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
278	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
277	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
276	Structure and Bonding Investigation of Plutonium Peroxocarbonate Complexes Using Cerium Surrogates and Electronic Structure Modeling. *Inorganic Chemistry*, **2017**, 56, 791-801	5.1	13
275	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
274	Enantioselective Recognition of Ammonium Carbamates in a Chiral Metal-Organic Framework. *Journal of the American Chemical Society*, **2017**, 139, 16000-16012	16.4	61
273	A new Pu(iii) coordination geometry in (CHNBr)[PuCl(HO)]2Cl2HO as obtained via supramolecular assembly in aqueous, high chloride media. *Chemical Communications*, **2017**, 53, 10816-10819	5.8	6
272	Engaging the Terminal: Promoting Halogen Bonding Interactions with Uranyl Oxo Atoms. *Chemistry - A European Journal*, **2017**, 23, 15355-15369	4.8	32
271	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
270	The unexpected roles of and 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

269	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
268	Electronic □to-□ Excitations of Rhodamine Dyes Exhibit a Time-Dependent Kohn-Sham Theory "Cyanine Problem". *ChemistryOpen*, **2017**, 6, 385-392	2.3	18
267	Electronic Structure and Properties of Berkelium Iodates. *Journal of the American Chemical Society*, **2017**, 139, 13361-13375	16.4	18
266	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
265	X-ray circular dichroism signals: a unique probe of local molecular chirality. *Chemical Science*, **2017**, 8, 5969-5978	9.4	15
264	Transuranic Hybrid Materials: Crystallographic and Computational Metrics of Supramolecular Assembly. *Journal of the American Chemical Society*, **2017**, 139, 10843-10855	16.4	39
263	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
262	Relativistic Methods for Calculating Electron Paramagnetic Resonance (EPR) Parameters **2017**, 725-763		8
261	Relativistic Theories of NMR Shielding **2017**, 657-692		9
260	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
259	Characterization of berkelium(III) dipicolinate and borate compounds in solution and the solid state. *Science*, **2016**, 353,	33.3	73
258	Ionic Liquid Solvation versus Catalysis: Computational Insight from a Multisubstituted Imidazole Synthesis in [EtNH][HSO]. *ChemistryOpen*, **2016**, 5, 460-469	2.3	17
257	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
256	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
255	A Nonorthogonal State-Interaction Approach for Matrix Product State Wave Functions. *Journal of Chemical Theory and Computation*, **2016**, 12, 5881-5894	6.4	26
254	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
253	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
252	Electronic and chiroptical properties of chiral cycloiridiated complexes bearing helicenic NHC ligands. *Chemical Communications*, **2016**, 52, 9243-6	5.8	22

251	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
250	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
249	Conformational changes and chiroptical switching of enantiopure bis-helicenic terpyridine upon Zn(2+) binding. *Chemical Communications*, **2016**, 52, 5932-5	5.8	69
248	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	6.4	16
247	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
246	Orbitals for Analyzing Bonding and Magnetism of Heavy-Metal Complexes. *Comments on Inorganic Chemistry*, **2016**, 36, 215-244	3.9	23
245	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
244	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
243	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
242	Calculated Resonance Vibrational Raman Optical Activity Spectra of Naproxen and Ibuprofen. *Journal of Physical Chemistry A*, **2016**, 120, 9740-9748	2.8	14
241	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, **2016**, 37, 506-41	3.5	1047
240	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
239	Nuclear Magnetic Resonance Measurements and Electronic Structure of Pu(IV) in [(Me)4N]2PuCl6. *Inorganic Chemistry*, **2016**, 55, 8371-80	5.1	14
238	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
237	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
236	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
235	Computational Tools for Predictive Modeling of Properties in Complex Actinide Systems **2015**, 299-342		2
234	Relativistic Methods for Calculating Electron Paramagnetic Resonance (EPR) Parameters **2015**, 1-39		2

233	Single-ion 4f element magnetism: an ab-initio look at Ln(COT)2(-). *Dalton Transactions*, **2015**, 44, 19886-909	4.9	45
232	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
231	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
230	Ruthenium-Grafted Vinylhelicenes: Chiroptical Properties and Redox Switching. *Chemistry - A European Journal*, **2015**, 21, 17100-15	4.8	38
229	Temperature dependence of contact and dipolar NMR chemical shifts in paramagnetic molecules. *Journal of Chemical Physics*, **2015**, 142, 054108	3.9	51
228	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
227	Charge-Transfer Versus Charge-Transfer-Like Excitations Revisited. *Journal of Chemical Theory and Computation*, **2015**, 11, 3305-20	6.4	62
226	Calculating NMR Chemical Shifts for Paramagnetic Metal Complexes from First-Principles. *Journal of Physical Chemistry Letters*, **2015**, 6, 2183-8	6.4	52
225	NMR Calculations for Paramagnetic Molecules and Metal Complexes. *Annual Reports in Computational Chemistry*, **2015**, 11, 3-36	1.8	15
224	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
223	enantio-Enriched CPL-active helicene-bipyridine-rhenium complexes. *Chemical Communications*, **2015**, 51, 3754-7	5.8	70
222	Relativistic Theories of NMR Shielding **2015**, 1-33		2
221	Calculation of nuclear spin-spin coupling constants using frozen density embedding. *Journal of Chemical Physics*, **2014**, 140, 104107	3.9	8
220	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
219	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
218	Electronic Energy Gaps for Conjugated Oligomers and Polymers Calculated with Density Functional Theory. *Journal of Chemical Theory and Computation*, **2014**, 10, 1035-47	6.4	111
217	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
216	Unravelling the structure of Magnus' pink salt. *Journal of the American Chemical Society*, **2014**, 136, 1333-51	11.4	55

215	Electronic Band Shapes Calculated with Optimally Tuned Range-Separated Hybrid Functionals. *Journal of Chemical Theory and Computation*, **2014**, 10, 4599-608	6.4	36
214	Helicene-grafted vinyl- and carbene-osmium complexes: an example of acid-base chiroptical switching. *Chemical Communications*, **2014**, 50, 2854-6	5.8	33
213	Magnetic resonance properties of actinyl carbonate complexes and plutonyl(VI)-tris-nitrate. *Inorganic Chemistry*, **2014**, 53, 8577-92	5.1	39
212	An investigation of chlorine ligands in transition-metal complexes via Cl solid-state NMR and density functional theory calculations. *Inorganic Chemistry*, **2014**, 53, 9581-97	5.1	21
211	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
210	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
209	Delocalization error and "functional tuning" in Kohn-Sham calculations of molecular properties. *Accounts of Chemical Research*, **2014**, 47, 2592-602	24.3	196
208	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
207	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
206	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
205	Calculating NMR Chemical Shifts and J-Couplings for Heavy Element Compounds **2014**, 1-14		3
204	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
203	Magnetic properties and electronic structures of Ar3U(IV) Complexes with Ar = C5(CH3)4H or C5H5 and L = CH3, NO, and Cl. *Inorganic Chemistry*, **2014**, 53, 13174-87	5.1	26
202	Relativistic Effects on NMR Parameters. *Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems*, **2013**, 3, 69-117		25
201	Chiroptical properties of carbo[6]helicene derivatives bearing extended conjugated cyano substituents. *Chirality*, **2013**, 25, 455-65	2.1	31
200	Giant Faraday Rotation in Mesogenic Organic Molecules. *Chemistry of Materials*, **2013**, 25, 1139-1143	9.6	35
199	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
198	Determination of the structures of molecularly imprinted polymers and xerogels using an automated stochastic approach. *Analytical Chemistry*, **2013**, 85, 8577-84	7.8	8

197	Spirooxazine-based multifunctional molecular switches with tunable photochromism and nonlinear optical response. *Journal of Materials Chemistry C*, **2013**, 1, 5779	7.1	20
196	Calculating Electronic Optical Activity of Coordination Compounds **2013**, 407-426		10
195	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
194	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
193	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
192	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
191	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
190	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
189	Computational Modeling of the Optical Rotation of Amino Acids: An In Silico Experiment for Physical Chemistry. *Journal of Chemical Education*, **2013**, 90, 656-660	2.4	12
188	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
187	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
186	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
185	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
184	Direct spectroscopic characterization of a transitory dirhodium donor-acceptor carbene complex. *Science*, **2013**, 342, 351-4	33.3	146
183	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
182	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
181	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
180	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

179	Curvature and Frontier Orbital Energies in Density Functional Theory. *Journal of Physical Chemistry Letters*, **2012**, 3, 3740-4	6.4	134
178	AB Initio Electronic Circular Dichroism and Optical Rotatory Dispersion: From Organic Molecules to Transition Metal Complexes **2012**, 593-642		15
177	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
176	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
175	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
174	Time-dependent density functional methods for surface enhanced Raman scattering (SERS) studies. *Computational and Theoretical Chemistry*, **2012**, 987, 32-41	2	19
173	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
172	Density functional study of tetraphenylporphyrin long-range exciton coupling. *ChemistryOpen*, **2012**, 1, 184-94	2.3	18
171	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
170	Quasiparticle spectra from a nonempirical optimally tuned range-separated hybrid density functional. *Physical Review Letters*, **2012**, 109, 226405	7.4	203
169	Orbitals: Some Fiction and Some Facts. *Journal of Chemical Education*, **2012**, 89, 1032-1040	2.4	35
168	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
167	Perspective: relativistic effects. *Journal of Chemical Physics*, **2012**, 136, 150902	3.9	189
166	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
165	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
164	Solvent effects and dynamic averaging of 195Pt NMR shielding in cisplatin derivatives. *Inorganic Chemistry*, **2011**, 50, 1723-32	5.1	54
163	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
162	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

161	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
160	[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
159	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
158	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
157	Tetracycline speciation during molecular imprinting in xerogels results in class-selective binding. *Analyst, The*, **2011**, 136, 749-55	5	18
156	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
155	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
154	Optical rotation calculated with time-dependent density functional theory: the OR45 benchmark. *Journal of Physical Chemistry A*, **2011**, 115, 10930-49	2.8	97
153	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
152	NMR J-coupling constants in cisplatin derivatives studied by molecular dynamics and relativistic DFT. *ChemPhysChem*, **2011**, 12, 1448-55	3.2	22
151	Time-dependent density functional theory for calculating origin-independent optical rotation and rotatory strength tensors. *ChemPhysChem*, **2011**, 12, 3224-35	3.2	60
150	Rhodium(II)-Catalyzed Cross-Coupling of Diazo Compounds. *Angewandte Chemie*, **2011**, 123, 2592-2596	3.6	35
149	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
148	Rhodium(II)-catalyzed cross-coupling of diazo compounds. *Angewandte Chemie - International Edition*, **2011**, 50, 2544-8	16.4	87
147	(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
146	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
145	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
144	Time-dependent density functional response theory for electronic chiroptical properties of chiral molecules. *Topics in Current Chemistry*, **2011**, 298, 1-98		84

143	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
142	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
141	Synthesis and evaluation of tetracycline imprinted xerogels: comparison of experiment and computational modeling. *Analytica Chimica Acta*, **2011**, 684, 63-71	6.6	19
140	Calculating the Raman and HyperRaman Spectra of Large Molecules and Molecules Interacting with Nanoparticles **2011**, 493-514		
139	Theoretical studies of surface enhanced hyper-Raman spectroscopy: the chemical enhancement mechanism. *Journal of Chemical Physics*, **2010**, 133, 054103	3.9	40
138	Analyzing molecular static linear response properties with perturbed localized orbitals. *Journal of Chemical Physics*, **2010**, 133, 044109	3.9	17
137	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
136	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
135	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
134	Electronic structure and circular dichroism of tris(bipyridyl) metal complexes within density functional theory. *Inorganic Chemistry*, **2010**, 49, 1355-62	5.1	40
133	Novel pathways for enhancing nonlinearity of organics utilizing metal clusters. *Journal of Physical Chemistry A*, **2010**, 114, 7590-4	2.8	17
132	Microscopic cascading of second-order molecular nonlinearity: New design principles for enhancing third-order nonlinearity. *Optics Express*, **2010**, 18, 8713-21	3.3	14
131	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
130	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
129	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
128	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
127	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
126	Metallahelicenes: Easily Accessible Helicene Derivatives with Large and Tunable Chiroptical Properties. *Angewandte Chemie*, **2010**, 122, 103-106	3.6	40

125	Metallahelicenes: easily accessible helicene derivatives with large and tunable chiroptical properties. *Angewandte Chemie - International Edition*, **2010**, 49, 99-102	16.4	126
124	Molecular orbital analysis of the inverse halogen dependence of nuclear magnetic shielding in LaX_3, X = F, Cl, Br, I. *Magnetic Resonance in Chemistry*, **2010**, 48 Suppl 1, S76-85	2.1	21
123	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
122	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
121	Computing chiroptical properties with first-principles theoretical methods: background and illustrative examples. *Chirality*, **2009**, 21 Suppl 1, E116-52	2.1	264
120	Charge-transfer excitations and time-dependent density functional theory: problems and some proposed solutions. *ChemPhysChem*, **2009**, 10, 1757-60	3.2	167
119	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
118	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
117	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
116	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
115	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
114	Computational study on the selectivity of donor/acceptor-substituted rhodium carbenoids. *Journal of Organic Chemistry*, **2009**, 74, 6555-63	4.2	154
113	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
112	A New Reaction for Organoselenium Compounds: Alkyl Transfer from Diorganoselenium(IV) Dibromides to Alkenoic Acids To Give γ- and δ-Lactones. *Organometallics*, **2009**, 28, 3426-3436	3.8	22
111	Solid-state chlorine NMR of group IV transition metal organometallic complexes. *Journal of the American Chemical Society*, **2009**, 131, 3317-30	16.4	79
110	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
109	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
108	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

107	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
106	Spectroscopic Properties Obtained from Time-Dependent Density Functional Theory (TD-DFT) **2009**,		1
105	Paramagnetic effects on the NMR spectra of "diamagnetic" ruthenium(bis-phosphine)(bis-semiquinone) complexes. *Inorganic Chemistry*, **2009**, 48, 5504-11	5.1	25
104	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
103	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
102	Enhancement of IR and VCD intensities due to charge transfer. *Physical Chemistry Chemical Physics*, **2009**, 11, 1526-38	3.6	50
101	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
100	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
99	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
98	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
97	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
96	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
95	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
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	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
92	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
91	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
90	A revised electronic Hessian for approximate time-dependent density functional theory. *Journal of Chemical Physics*, **2008**, 129, 184114	3.9	62

89	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
88	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
87	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
86	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
85	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
84	A pragmatic recipe for the treatment of hindered rotations in the vibrational averaging of molecular properties. *ChemPhysChem*, **2008**, 9, 159-70	3.2	34
83	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
82	Vibrational corrections to magneto-optical rotation: a computational study. *Journal of Physical Chemistry A*, **2007**, 111, 5563-71	2.8	10
81	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
80	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
79	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
78	Relativistic Computation of NMR Shieldings and Spin-Spin Coupling Constants **2007**,		2
77	Analyzing and Interpreting NMR Spin–Spin Coupling Constants Using Molecular Orbital Calculations. *Journal of Chemical Education*, **2007**, 84, 156	2.4	61
76	Density Functional Studies of the 13C NMR Chemical Shifts in Single-Walled Carbon Nanotubes. *AIP Conference Proceedings*, **2007**,	0	1
75	Downfolding and N-ization of Basis Sets of Slater Type Orbitals. *AIP Conference Proceedings*, **2007**,	0	1
74	Temperature dependence of the optical rotation in six bicyclic organic molecules calculated by vibrational averaging. *ChemPhysChem*, **2007**, 8, 605-16	3.2	28
73	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
72	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

71	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
70	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
69	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
68	Computation of Optical Rotation using Time-Dependent Density Functional Theory. *Computing Letters*, **2007**, 3, 131-150		37
67	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
66	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
65	Resonance vibrational Raman optical activity: a time-dependent density functional theory approach. *Journal of Chemical Physics*, **2007**, 127, 134101	3.9	68
64	A quantum chemical approach to the design of chiral negative index materials. *Optics Express*, **2007**, 15, 5730-41	3.3	45
63	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
62	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
61	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
60	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
59	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
58	DFT Calculations of the 183W NMR Chemical Shifts in Reduced Polyoxotungstates. *European Journal of Inorganic Chemistry*, **2006**, 2006, 1149-1154	2.3	25
57	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
56	Magic alkali-fullerene compound clusters of extreme thermal stability. *Journal of Chemical Physics*, **2006**, 125, 191102	3.9	10
55	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
54	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

53	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
52	Temperature dependence of the optical rotation of fenchone calculated by vibrational averaging. *Journal of Physical Chemistry A*, **2006**, 110, 11381-3	2.8	35
51	Spectral and structural characterization of amidate-bridged platinum-thallium complexes with strong metal-metal bonds. *Inorganic Chemistry*, **2006**, 45, 4526-36	5.1	50
50	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
49	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
48	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
47	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
46	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
45	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
44	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
43	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
42	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
41	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
40	Theoretical methods of potential use for studies of inorganic reaction mechanisms. *Chemical Reviews*, **2005**, 105, 2695-722	68.1	364
39	Finite lifetime effects on the polarizability within time-dependent density-functional theory. *Journal of Chemical Physics*, **2005**, 122, 224115	3.9	146
38	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
37	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
36	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

35	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
34	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
33	Ab initio calculation of the C/D ratio of magnetic circular dichroism. *Journal of Chemical Physics*, **2005**, 122, 094112	3.9	29
32	Theory and method for calculating resonance Raman scattering from resonance polarizability derivatives. *Journal of Chemical Physics*, **2005**, 123, 174110	3.9	155
31	Importance of vibronic effects on the circular dichroism spectrum of dimethyloxirane. *Journal of Chemical Physics*, **2005**, 122, 234305	3.9	52
30	Relativistic Calculations of Spin□pin Coupling Constants of Heavy Nuclei **2004**, 249-264		30
29	Calculation of Heavy-Nucleus Chemical Shifts. Relativistic All-Electron Methods **2004**, 227-247		34
28	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
27	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
26	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
25	Properties of WAu12. *Physical Chemistry Chemical Physics*, **2004**, 6, 11-22	3.6	93
24	The Calculation of NMR Parameters in Transition Metal Complexes. *Structure and Bonding*, **2004**, 1-48	0.9	64
23	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
22	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
21	Double perturbation theory: a powerful tool in computational coordination chemistry. *Coordination Chemistry Reviews*, **2003**, 238-239, 83-126	23.2	86
20	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
19	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
18	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

17	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
16	Density functional calculations on electronic circular dichroism spectra of chiral transition metal complexes. *Inorganic Chemistry*, **2003**, 42, 2867-77	5.1	86
15	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
14	Relativistic Density-Functional Computations of the Chemical Shift of 129Xe in . *Journal of Physical Chemistry A*, **2003**, 107, 4967-4972	2.8	59
13	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
12	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
11	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
10	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
9	Calculating molecular electric and magnetic properties from time-dependent density functional response theory. *Journal of Chemical Physics*, **2002**, 116, 891-896	3.9	86
8	199Hg Shielding Tensor in Methylmercury Halides: NMR Experiments and ZORA DFT Calculations. *Journal of Physical Chemistry A*, **2002**, 106, 9313-9318	2.8	33
7	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
6	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
5	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
4	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
3	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
2	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
1	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