Michal Repisky

List of Publications by Year
in descending order

61	2,221	218677	223800
papers	citations	26	46
		h-index	g-index

63	63	63	1591
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A fully relativistic method for calculation of nuclear magnetic shielding tensors with a restricted magnetically balanced basis in the framework of the matrix Dirac–Kohn–Sham equation. Journal of Chemical Physics, 2008, 128, 104101.	3.0	196
2	Fully relativistic calculations of NMR shielding tensors using restricted magnetically balanced basis and gauge including atomic orbitals. Journal of Chemical Physics, 2010, 132, 154101.	3.0	141
3	Relativistic Four-Component DFT Calculations of ^{1}H NMR Chemical Shifts in Transition-Metal Hydride Complexes: Unusual High-Field Shifts Beyond the Buckingham–Stephens Model. Journal of Physical Chemistry A, 2011, 115, 5654-5659.	2.5	120
4	A Combined Atomic Force Microscopy and Computational Approach for the Structural Elucidation of Breitfussin A and B: Highly Modified Halogenated Dipeptides from *Thuiaria breitfussi*. Angewandte Chemie - International Edition, 2012, 51, 12238-12241.	13.8	92
5	ReSpect: Relativistic spectroscopy DFT program package. Journal of Chemical Physics, 2020, 152, 184101.	3.0	90
6	Structure, solvent, and relativistic effects on the NMR chemical shifts in square-planar transition-metal complexes: assessment of DFT approaches. Physical Chemistry Chemical Physics, 2015, 17, 24944-24955.	2.8	82
7	Effects of finite size nuclei in relativistic four-component calculations of hyperfine structure. Journal of Chemical Physics, 2011, 134, 044111.	3.0	72
8	Excitation Energies from Real-Time Propagation of the Four-Component Dirac–Kohn–Sham Equation. Journal of Chemical Theory and Computation, 2015, 11, 980-991.	5.3	72
9	The Absolute Shielding Constants of Heavy Nuclei: Resolving the Enigma of the ^{119}Sn Absolute Shielding. Journal of Physical Chemistry Letters, 2013, 4, 459-463.	4.6	64
10	Relativistic four-component calculations of electronic g-tensors in the matrix Dirac–Kohn–Sham framework. Chemical Physics Letters, 2010, 488, 94-97.	2.6	62
11	Restricted magnetically balanced basis applied for relativistic calculations of indirect nuclear spin–spin coupling tensors in the matrix Dirac–Kohn–Sham framework. Chemical Physics, 2009, 356, 236-242.	1.9	61
12	Four-Component Relativistic Density Functional Theory Calculations of NMR Shielding Tensors for Paramagnetic Systems. Journal of Physical Chemistry A, 2013, 117, 14209-14219.	2.5	60
13	X-ray absorption resonances near L$_{2,3}$-edges from real-time propagation of the Dirac–Kohn–Sham density matrix. Physical Chemistry Chemical Physics, 2015, 17, 22566-22570.	2.8	58
14	Linking the Character of the Metal–Ligand Bond to the Ligand NMR Shielding in Transition-Metal Complexes: NMR Contributions from Spin–Orbit Coupling. Journal of Chemical Theory and Computation, 2017, 13, 3586-3601.	5.3	55
15	Relativistic Spin–Orbit Heavy Atom on the Light Atom NMR Chemical Shifts: General Trends Across the Periodic Table Explained. Journal of Chemical Theory and Computation, 2018, 14, 3025-3039.	5.3	55
16	Dismutational and Global–Minimum Isomers of Heavier 1,4–Dimetallatetrasilabenzenes of Group 14. Angewandte Chemie - International Edition, 2014, 53, 3514-3518.	13.8	49
17	Four-Component Relativistic Density Functional Theory Calculations of EPR **g**- and Hyperfine-Coupling Tensors Using Hybrid Functionals: Validation on Transition-Metal Complexes with Large Tensor Anisotropies and Higher-Order Spin–Orbit Effects. Journal of Physical Chemistry A, 2015, 119, 12892-12905.	2.5	49
18	Acceleration of Relativistic Electron Dynamics by Means of X2C Transformation: Application to the Calculation of Nonlinear Optical Properties. Journal of Chemical Theory and Computation, 2016, 12, 5823-5833.	5.3	48

#	Article	IF	Citations
19	Resolution of identity Dirac-Kohn-Sham method using the large component only: Calculations of g-tensor and hyperfine tensor. Journal of Chemical Physics, 2006, 124, 084108.	3.0	41
20	Assessment of higher-order spin–orbit effects on electronic g-tensors of d 1 transition-metal complexes by relativistic two- and four-component methods. Theoretical Chemistry Accounts, 2011, 129, 715-725.	1.4	39
21	A comparison of two-component and four-component approaches for calculations of spin-spin coupling constants and NMR shielding constants of transition metal cyanides. Journal of Chemical Physics, 2012, 137, 014311.	3.0	34
22	Dinitrogen-Facilitated Reversible Formation of a Si–H Bond in a Pincer-Supported Ni Complex. Organometallics, 2016, 35, 3154-3162.	2.3	33
23	Four-component relativistic time-dependent density-functional theory using a stable noncollinear DFT ansatz applicable to both closed- and open-shell systems. Journal of Chemical Physics, 2019, 151, 184111.	3.0	33
24	Four-Component Relativistic Density-Functional Theory Calculations of Nuclear Spin–Rotation Constants: Relativistic Effects in p-Block Hydrides. Journal of Chemical Theory and Computation, 2015, 11, 3729-3739.	5.3	32
25	Understanding the Solution and Solid-State Structures of Pd and Pt PSiP Pincer-Supported Hydrides. Inorganic Chemistry, 2015, 54, 11411-11422.	4.0	31
26	Four–Component Relativistic DFT Calculations of ^{13}C Chemical Shifts of Halogenated Natural Substances. Chemistry - A European Journal, 2015, 21, 18834-18840.	3.3	27
27	Communication: The absolute shielding scales of oxygen and sulfur revisited. Journal of Chemical Physics, 2015, 142, 091102.	3.0	27
28	Relativistic Calculations of Nuclear Magnetic Resonance Parameters. New Developments in NMR, 2016, , 267-303.	0.1	26
29	Spin-rotation and NMR shielding constants in HCl. Journal of Chemical Physics, 2013, 139, 234302.	3.0	25
30	All-electron fully relativistic Kohn-Sham theory for solids based on the Dirac-Coulomb Hamiltonian and Gaussian-type functions. Physical Review B, 2019, 99, .	3.2	24
31	Resolution-of-identity accelerated relativistic two- and four-component electron dynamics approach to chiroptical spectroscopies. Journal of Chemical Physics, 2018, 149, 204104.	3.0	23
32	Four-component relativistic density functional theory with the polarisable continuum model: application to EPR parameters and paramagnetic NMR shifts. Molecular Physics, 2017, 115, 214-227.	1.7	21
33	Rovibrational Corrections to Transition Metal NMR Shielding Constants. ChemPhysChem, 2004, 5, 410-414.	2.1	20
34	How does relativity affect magnetically induced currents?. Chemical Communications, 2015, 51, 13961-13963.	4.1	20
35	Dinuclear fluoro-peroxovanadium(v) complexes with symmetric and asymmetric peroxo bridges: syntheses, structures and DFT studies. Dalton Transactions, 2009, , 465-473.	3.3	19
36	Four–component relativistic chemical shift calculations of halogenated organic compounds. Journal of Physical Organic Chemistry, 2013, 26, 679-687.	1.9	19

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37	Absolute NMR shielding scales and nuclear spin–rotation constants in 175LuX and 197AuX (X = 19F,) Tj ETQq1 1 0.784314 rgBT /C	3.0	18
38	Four-component relativistic ^{31}P NMR calculations for *trans*-platinum(ii) complexes: importance of the solvent and dynamics in spectral simulations. Dalton Transactions, 2019, 48, 8076-8083.	3.3	18
39	Generalization of Intrinsic Orbitals to Kramers-Paired Quaternion Spinors, Molecular Fragments, and Valence Virtual Spinors. Journal of Chemical Theory and Computation, 2021, 17, 1337-1354.	5.3	18
40	Experimental and four‐component relativistic DFT studies of tungsten carbonyl complexes. Journal of Physical Organic Chemistry, 2015, 28, 723-731.	1.9	17
41	Relativistic four-component linear damped response TDDFT for electronic absorption and circular dichroism calculations. Journal of Chemical Physics, 2019, 151, 194112.	3.0	17
42	Implementation of Relativistic Coupled Cluster Theory for Massively Parallel GPU-Accelerated Computing Architectures. Journal of Chemical Theory and Computation, 2021, 17, 5509-5529.	5.3	17
43	Relativistic DFT Calculations of Hyperfine Coupling Constants in 5d Hexafluorido Complexes: [ReF$_6$]$^{2−}$ and [IrF$_6$]$^{2−}$. Chemistry - A European Journal, 2018, 24, 5124-5133.	3.3	16
44	Relativistic four-component calculations of indirect nuclear spin-spin couplings with efficient evaluation of the exchange-correlation response kernel. Journal of Chemical Physics, 2015, 142, 114102.	3.0	15
45	Interplay of Through-Bond Hyperfine and Substituent Effects on the NMR Chemical Shifts in Ru(III) Complexes. Inorganic Chemistry, 2018, 57, 8748-8759.	4.0	14
46	Cob(II)alamin: Relativistic DFT Analysis of the EPR Parameters. Journal of Chemical Theory and Computation, 2014, 10, 2125-2136.	5.3	12
47	First-Principles Calculation of ^{1}H NMR Chemical Shifts of Complex Metal Polyhydrides: The Essential Inclusion of Relativity and Dynamics. Inorganic Chemistry, 2020, 59, 17509-17518.	4.0	12
48	Accurate X-ray Absorption Spectra near L- and M-Edges from Relativistic Four-Component Damped Response Time-Dependent Density Functional Theory. Inorganic Chemistry, 2022, 61, 830-846.	4.0	12
49	Probing Structure in the Polymorphic Domain of the l-Enantiomer of N-Benzoyl-Phenylalanine by Means of 2D Solid-State NMR Spectroscopy and DFT Calculations. Journal of Physical Chemistry B, 2005, 109, 23175-23182.	2.6	11
50	Relativistic Cholesky-decomposed density matrix MP2. Chemical Physics, 2019, 518, 38-46.	1.9	11
51	NMR Spin–Spin Coupling Constants Derived from Relativistic Four-Component DFT Theory—Analysis and Visualization. Journal of Physical Chemistry A, 2020, 124, 5157-5169.	2.5	10
52	Implementation of the diagonalization‐free algorithm in the self‐consistent field procedure within the four‐component relativistic scheme. Journal of Computational Chemistry, 2014, 35, 1725-1737.	3.3	8
53	Nuclear magnetic dipole moment of ^{209}Bi from NMR experiments. Physical Review A, 2018, 98, .	2.5	8
54	Laplace-transformed atomic orbital-based Møller–Plesset perturbation theory for relativistic two-component Hamiltonians. Journal of Chemical Physics, 2016, 145, 014107.	3.0	7

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55	Indirect NMR spin–spin coupling constants in diatomic alkali halides. Journal of Chemical Physics, 2016, 145, 244308.	3.0	7
56	New quantum number for the many-electron Dirac-Coulomb Hamiltonian. Physical Review A, 2016, 94, .	2.5	6
57	Electron and nuclear spin polarization in Rb-Xe spin-exchange optical hyperpolarization. Physical Review A, 2017, 95, .	2.5	6
58	NMR absolute shielding scales and nuclear magnetic dipole moments of transition metal nuclei. Physical Chemistry Chemical Physics, 2020, 22, 7065-7076.	2.8	6
59	Supramolecular Coronation of Platinum(II) Complexes by Macrocycles: Structure, Relativistic DFT Calculations, and Biological Effects. Inorganic Chemistry, 2021, 60, 17911-17925.	4.0	5
60	Fully relativistic calculations of NMR and EPR parameters in the framework of the matrix Dirac-Kohn-Sham equation. AIP Conference Proceedings, 2012, , .	0.4	1
61	Frontispiece: Relativistic DFT Calculations of Hyperfine Coupling Constants in 5d Hexafluorido Complexes: [ReF6]2⁻ and [IrF6]2⁻. Chemistry - A European Journal, 2018, 24, .	3.3	1