Michal Repisky

List of Publications by Year
in descending order

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

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

#	Article	IF	Citations
1	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
2	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
3	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
4	Supramolecular Coronation of Platinum(II) Complexes by Macrocycles: Structure, Relativistic DFT Calculations, and Biological Effects. Inorganic Chemistry, 2021, 60, 17911-17925.	4.0	5
5	First-Principles Calculation of ¹H NMR Chemical Shifts of Complex Metal Polyhydrides: The Essential Inclusion of Relativity and Dynamics. Inorganic Chemistry, 2020, 59, 17509-17518.	4.0	12
6	ReSpect: Relativistic spectroscopy DFT program package. Journal of Chemical Physics, 2020, 152, 184101.	3.0	90
7	NMR Spinâ€“Spin Coupling Constants Derived from Relativistic Four-Component DFT Theoryâ€”Analysis and Visualization. Journal of Physical Chemistry A, 2020, 124, 5157-5169.	2.5	10
8	NMR absolute shielding scales and nuclear magnetic dipole moments of transition metal nuclei. Physical Chemistry Chemical Physics, 2020, 22, 7065-7076.	2.8	6
9	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
10	Four-component relativistic ³¹P NMR calculations for trans-platinum(<scp>ii</scp>) complexes: importance of the solvent and dynamics in spectral simulations. Dalton Transactions, 2019, 48, 8076-8083.	3.3	18
11	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
12	Relativistic four-component linear damped response TDDFT for electronic absorption and circular dichroism calculations. Journal of Chemical Physics, 2019, 151, 194112.	3.0	17
13	Relativistic Cholesky-decomposed density matrix MP2. Chemical Physics, 2019, 518, 38-46.	1.9	11
14	Relativistic Spinâ€“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
15	Frontispiece: Relativistic DFT Calculations of Hyperfine Coupling Constants in 5d Hexafluorido Complexes: [ReF6]2â^' and [IrF6]2â^'. Chemistry - A European Journal, 2018, 24, .	3.3	1
16	Relativistic DFT Calculations of Hyperfine Coupling Constants in 5d Hexafluorido Complexes: [ReF₆]^{2â^'} and [IrF₆]^{2â^'}. Chemistry - A European Journal, 2018, 24, 5124-5133.	3.3	16
17	Nuclear magnetic dipole moment of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mmultiscripts><mml:mi>Bi</mml:mi><mml:mprescripts /><mml:none /><mml:mn>209</mml:mn></mml:mmultiscripts></mml:math> from NMR experiments. Physical Review A, 2018, 98, .	2.5	8
18	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

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19	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
20	Electron and nuclear spin polarization in Rb-Xe spin-exchange optical hyperpolarization. Physical Review A, 2017, 95, .	2.5	6
21	Linking the Character of the Metalâ€“Ligand Bond to the Ligand NMR Shielding in Transition-Metal Complexes: NMR Contributions from Spinâ€“Orbit Coupling. Journal of Chemical Theory and Computation, 2017, 13, 3586-3601.	5.3	55
22	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
23	Laplace-transformed atomic orbital-based MÃ¸llerâ€“Plesset perturbation theory for relativistic two-component Hamiltonians. Journal of Chemical Physics, 2016, 145, 014107.	3.0	7
24	Indirect NMR spinâ€“spin coupling constants in diatomic alkali halides. Journal of Chemical Physics, 2016, 145, 244308.	3.0	7
25	New quantum number for the many-electron Dirac-Coulomb Hamiltonian. Physical Review A, 2016, 94, .	2.5	6
26	Dinitrogen-Facilitated Reversible Formation of a Siâ€“H Bond in a Pincer-Supported Ni Complex. Organometallics, 2016, 35, 3154-3162.	2.3	33
27	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
28	Relativistic Calculations of Nuclear Magnetic Resonance Parameters. New Developments in NMR, 2016, , 267-303.	0.1	26
29	Absolute NMR shielding scales and nuclear spinâ€“rotation constants in 175LuX and 197AuX (X = 19F,) Tj ETQq1 1 0.784314 rgBT /Ov	3.0	18
30	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
31	Experimental and fourâ€component relativistic DFT studies of tungsten carbonyl complexes. Journal of Physical Organic Chemistry, 2015, 28, 723-731.	1.9	17
32	Fourâ€Component Relativistic DFT Calculations of ¹³C Chemical Shifts of Halogenated Natural Substances. Chemistry - A European Journal, 2015, 21, 18834-18840.	3.3	27
33	Four-Component Relativistic Density Functional Theory Calculations of EPRg- and Hyperfine-Coupling Tensors Using Hybrid Functionals: Validation on Transition-Metal Complexes with Large Tensor Anisotropies and Higher-Order Spinâ€“Orbit Effects. Journal of Physical Chemistry A, 2015, 119, 12892-12905.	2.5	49
34	Understanding the Solution and Solid-State Structures of Pd and Pt PSiP Pincer-Supported Hydrides. Inorganic Chemistry, 2015, 54, 11411-11422.	4.0	31
35	Excitation Energies from Real-Time Propagation of the Four-Component Diracâ€“Kohnâ€“Sham Equation. Journal of Chemical Theory and Computation, 2015, 11, 980-991.	5.3	72
36	Four-Component Relativistic Density-Functional Theory Calculations of Nuclear Spinâ€“Rotation Constants: Relativistic Effects in p-Block Hydrides. Journal of Chemical Theory and Computation, 2015, 11, 3729-3739.	5.3	32

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37	How does relativity affect magnetically induced currents?. Chemical Communications, 2015, 51, 13961-13963.	4.1	20
38	X-ray absorption resonances near L_{2,3}-edges from real-time propagation of the Diracâ€“Kohnâ€“Sham density matrix. Physical Chemistry Chemical Physics, 2015, 17, 22566-22570.	2.8	58
39	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
40	Communication: The absolute shielding scales of oxygen and sulfur revisited. Journal of Chemical Physics, 2015, 142, 091102.	3.0	27
41	Dismutational and Globalâ€Minimum Isomers of Heavier 1,4â€Dimetallatetrasilabenzenes of Groupâ€...14. Angewandte Chemie - International Edition, 2014, 53, 3514-3518.	13.8	49
42	Cob(II)alamin: Relativistic DFT Analysis of the EPR Parameters. Journal of Chemical Theory and Computation, 2014, 10, 2125-2136.	5.3	12
43	Implementation of the diagonalizationâ€free algorithm in the selfâ€consistent field procedure within the fourâ€component relativistic scheme. Journal of Computational Chemistry, 2014, 35, 1725-1737.	3.3	8
44	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
45	The Absolute Shielding Constants of Heavy Nuclei: Resolving the Enigma of the ¹¹⁹Sn Absolute Shielding. Journal of Physical Chemistry Letters, 2013, 4, 459-463.	4.6	64
46	Fourâ€component relativistic chemical shift calculations of halogenated organic compounds. Journal of Physical Organic Chemistry, 2013, 26, 679-687.	1.9	19
47	Spin-rotation and NMR shielding constants in HCl. Journal of Chemical Physics, 2013, 139, 234302.	3.0	25
48	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
49	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
50	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
51	Relativistic Four-Component DFT Calculations of ¹H NMR Chemical Shifts in Transition-Metal Hydride Complexes: Unusual High-Field Shifts Beyond the Buckinghamâ€“Stephens Model. Journal of Physical Chemistry A, 2011, 115, 5654-5659.	2.5	120
52	Assessment of higher-order spinâ€“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
53	Effects of finite size nuclei in relativistic four-component calculations of hyperfine structure. Journal of Chemical Physics, 2011, 134, 044111.	3.0	72
54	Relativistic four-component calculations of electronic g-tensors in the matrix Diracâ€“Kohnâ€“Sham framework. Chemical Physics Letters, 2010, 488, 94-97.	2.6	62

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55	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
56	Restricted magnetically balanced basis applied for relativistic calculations of indirect nuclear spinâ€“spin coupling tensors in the matrix Diracâ€“Kohnâ€“Sham framework. Chemical Physics, 2009, 356, 236-242.	1.9	61
57	Dinuclear fluoro-peroxovanadium(v) complexes with symmetric and asymmetric peroxo bridges: syntheses, structures and DFT studies. Dalton Transactions, 2009, , 465-473.	3.3	19
58	A fully relativistic method for calculation of nuclear magnetic shielding tensors with a restricted magnetically balanced basis in the framework of the matrix Diracâ€“Kohnâ€“Sham equation. Journal of Chemical Physics, 2008, 128, 104101.	3.0	196
59	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
60	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
61	Rovibrational Corrections to Transition Metal NMR Shielding Constants. ChemPhysChem, 2004, 5, 410-414.	2.1	20