

Wenjian Liu

List of Publications by Year in descending order

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155
papers

7,569
citations

31976

53
h-index

60623

81
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166
docs citations

166
times ranked

3354
citing authors

#	ARTICLE	IF	CITATIONS
1	Quasirelativistic theory equivalent to fully relativistic theory. <i>Journal of Chemical Physics</i> , 2005, 123, 241102.	3.0	398
2	Exact two-component Hamiltonians revisited. <i>Journal of Chemical Physics</i> , 2009, 131, 031104.	3.0	298
3	Ideas of relativistic quantum chemistry. <i>Molecular Physics</i> , 2010, 108, 1679-1706.	1.7	286
4	The Beijing four-component density functional program package (BDF) and its application to EuO, EuS, YbO and YbS. <i>Theoretical Chemistry Accounts</i> , 1997, 96, 75-83.	1.4	247
5	Infinite-order quasirelativistic density functional method based on the exact matrix quasirelativistic theory. <i>Journal of Chemical Physics</i> , 2006, 125, 044102.	3.0	225
6	Making four- and two-component relativistic density functional methods fully equivalent based on the idea of "from atoms to molecule". <i>Journal of Chemical Physics</i> , 2007, 127, 104106.	3.0	210
7	The Beijing Density Functional (BDF) Program Package: Methodologies and Applications. <i>Journal of Theoretical and Computational Chemistry</i> , 2003, 02, 257-272.	1.8	157
8	Quasirelativistic theory. II. Theory at matrix level. <i>Journal of Chemical Physics</i> , 2007, 126, 114107.	3.0	149
9	Morphological effects of the nanostructured ceria support on the activity and stability of CuO/CeO ₂ catalysts for the water-gas shift reaction. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 17183-17195.	2.8	143
10	A small-core multiconfiguration Dirac-Hartree-Fock-adjusted pseudopotential for Tl - application to Tl X (X = F, Cl, Br, I). <i>Theoretical Chemistry Accounts</i> , 2000, 104, 22-28.	1.4	138
11	Unraveling the Dynamic Nature of a CuO/CeO ₂ Catalyst for CO Oxidation in <i>Operando</i> : A Combined Study of XANES (Fluorescence) and DRIFTS. <i>ACS Catalysis</i> , 2014, 4, 1650-1661.	11.2	128
12	On the spin separation of algebraic two-component relativistic Hamiltonians. <i>Journal of Chemical Physics</i> , 2012, 137, 154114.	3.0	123
13	iCI: Iterative CI toward full CI. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1169-1178.	5.3	123
14	Advances in relativistic molecular quantum mechanics. <i>Physics Reports</i> , 2014, 537, 59-89.	25.6	122
15	Quasirelativistic theory I. Theory in terms of a quasi-relativistic operator. <i>Molecular Physics</i> , 2006, 104, 2225-2240.	1.7	106
16	Rational Design of Photocatalysts for Controlled Polymerization: Effect of Structures on Photocatalytic Activities. <i>Chemical Reviews</i> , 2022, 122, 5476-5518.	47.7	106
17	Spectroscopic constants of gold and eka-gold (element 111) diatomic compounds: The importance of spin-orbit coupling. <i>Journal of Chemical Physics</i> , 1999, 110, 3730-3735.	3.0	100
18	Time-dependent four-component relativistic density functional theory for excitation energies. <i>Journal of Chemical Physics</i> , 2004, 121, 6658-6666.	3.0	94

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19	Time-dependent four-component relativistic density-functional theory for excitation energies. II. The exchange-correlation kernel. <i>Journal of Chemical Physics</i> , 2005, 123, 054102.	3.0	93
20	The Ground State Electronic Energy of Benzene. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 8922-8929.	4.6	90
21	Computer-Guided Discovery of a pH-Responsive Organic Photocatalyst and Application for pH and Light Dual-Gated Polymerization. <i>Journal of the American Chemical Society</i> , 2019, 141, 8207-8220.	13.7	89
22	Combining spin-adapted open-shell TD-DFT with spin-orbit coupling. <i>Molecular Physics</i> , 2013, 111, 3741-3755.	1.7	85
23	Four-component relativistic theory for nuclear magnetic shielding constants: Critical assessments of different approaches. <i>Journal of Chemical Physics</i> , 2007, 126, 214101.	3.0	83
24	First-order nonadiabatic coupling matrix elements between excited states: A Lagrangian formulation at the CIS, RPA, TD-HF, and TD-DFT levels. <i>Journal of Chemical Physics</i> , 2014, 141, 014110.	3.0	83
25	Four-component relativistic theory for nuclear magnetic shielding: Magnetically balanced gauge-including atomic orbitals. <i>Journal of Chemical Physics</i> , 2009, 131, 244113.	3.0	79
26	BDF: A relativistic electronic structure program package. <i>Journal of Chemical Physics</i> , 2020, 152, 064113.	3.0	79
27	Ab initio pseudopotential and density-functional all-electron study of ionization and excitation energies of actinide atoms. <i>Physical Review A</i> , 1998, 58, 1103-1110.	2.5	74
28	First order nonadiabatic coupling matrix elements between excited states: Implementation and application at the TD-DFT and pp-TDA levels. <i>Journal of Chemical Physics</i> , 2014, 141, 244105.	3.0	74
29	Comparison of restricted, unrestricted, inverse, and dual kinetic balances for four-component relativistic calculations. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 423-436.	1.4	73
30	Solvent Effects on the Optical Spectra and Excited-State Decay of Triphenylamine-thiadiazole with Hybridized Local Excitation and Intramolecular Charge Transfer. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5233-5240.	2.5	73
31	Performance of relativistic density functional and ab initio pseudopotential approaches for systems with high-spin multiplicities: Gadolinium diatomics GdX (X=H, N, O, F, P, S, Cl, Gd). <i>International Journal of Quantum Chemistry</i> , 2000, 76, 359-370.	2.0	72
32	Perspectives of relativistic quantum chemistry: the negative energy cat smiles. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 35-48.	2.8	72
33	Comparison of Different Polarization Schemes in Open-shell Relativistic Density Functional Calculations. <i>Journal of the Chinese Chemical Society</i> , 2003, 50, 597-606.	1.4	70
34	Linear-Scaling Time-Dependent Density Functional Theory Based on the Idea of "From Fragments to Molecule". <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3643-3660.	5.3	70
35	Spin-adapted open-shell random phase approximation and time-dependent density functional theory. I. Theory. <i>Journal of Chemical Physics</i> , 2010, 133, 064106.	3.0	68
36	Spin-adapted open-shell time-dependent density functional theory. II. Theory and pilot application. <i>Journal of Chemical Physics</i> , 2011, 134, 134101.	3.0	68

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37	Fully relativistic density functional calculations of the ground and excited states of Yb, YbH, YbF, and YbO. <i>Journal of Chemical Physics</i> , 1998, 108, 2886-2895.	3.0	67
38	On the spin separation of algebraic two-component relativistic Hamiltonians: Molecular properties. <i>Journal of Chemical Physics</i> , 2014, 141, 054111.	3.0	67
39	Iterative Configuration Interaction with Selection. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2296-2316.	5.3	67
40	Low-lying electronic states of lanthanocenes and actinocenes $M(C_8H_8)_2$ ($M=Nd, Tb, Yb, U$). <i>Journal of Chemical Physics</i> , 1997, 107, 3584-3591.	3.0	66
41	Theoretical and numerical assessments of spin-flip time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2012, 136, 024107.	3.0	66
42	Spectroscopic constants of Pb and Eka-lead compounds: comparison of different approaches. <i>Advances in Quantum Chemistry</i> , 2001, , 325-355.	0.8	65
43	Four-component relativistic theory for nuclear magnetic shielding constants: The orbital decomposition approach. <i>Journal of Chemical Physics</i> , 2007, 126, 081101.	3.0	64
44	Time-dependent quasirelativistic density-functional theory based on the zeroth-order regular approximation. <i>Journal of Chemical Physics</i> , 2005, 123, 144101.	3.0	63
45	Going beyond "no-pair relativistic quantum chemistry". <i>Journal of Chemical Physics</i> , 2013, 139, 014108.	3.0	63
46	SDS: the "static" "dynamic" "static"™ framework for strongly correlated electrons. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	1.4	61
47	Four-component relativistic theory for NMR parameters: Unified formulation and numerical assessment of different approaches. <i>Journal of Chemical Physics</i> , 2009, 130, 144102.	3.0	60
48	Spectroscopic constants of MH and M2 ($M=Tl, E113, Bi, E115$): Direct comparisons of four- and two-component approaches in the framework of relativistic density functional theory. <i>Journal of Chemical Physics</i> , 2002, 116, 3626-3634.	3.0	59
49	Spin-adapted open-shell time-dependent density functional theory. III. An even better and simpler formulation. <i>Journal of Chemical Physics</i> , 2011, 135, 194106.	3.0	57
50	Essentials of relativistic quantum chemistry. <i>Journal of Chemical Physics</i> , 2020, 152, 180901.	3.0	57
51	Exact two-component relativistic theory for nuclear magnetic resonance parameters. <i>Journal of Chemical Physics</i> , 2009, 131, 081101.	3.0	56
52	Benchmark calculations for lanthanide atoms: Calibration of ab initio and density-functional methods. <i>Physical Review A</i> , 1998, 57, 1721-1728.	2.5	55
53	Exact two-component relativistic theory for NMR parameters: General formulation and pilot application. <i>Journal of Chemical Physics</i> , 2012, 137, 174105.	3.0	54
54	Big picture of relativistic molecular quantum mechanics. <i>National Science Review</i> , 2016, 3, 204-221.	9.5	54

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55	Relativistic time-dependent density functional theories. <i>Chemical Society Reviews</i> , 2018, 47, 4481-4509.	38.1	54
56	Unravelling an oxygen-mediated reductive quenching pathway for photopolymerisation under long wavelengths. <i>Nature Communications</i> , 2021, 12, 478.	12.8	54
57	RELATIVISTIC DENSITY FUNCTIONAL THEORY: THE BDF PROGRAM PACKAGE. <i>Recent Advances in Computational</i> , 2004, , 257-282.	0.8	52
58	Fully relativistic theories and methods for NMR parameters. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	1.4	45
59	Calculated Properties of Lanthanocene Anions and the Unusual Electronic Structure of Their Neutral Counterparts. <i>Inorganic Chemistry</i> , 1998, 37, 1067-1072.	4.0	44
60	A spin-adapted size-extensive state-specific multi-reference perturbation theory. I. Formal developments. <i>Journal of Chemical Physics</i> , 2012, 136, 024105.	3.0	43
61	Relativistic ab initio and density functional theory calculations on the mercury fluorides: Is HgF ₄ thermodynamically stable?. <i>Chemical Physics Letters</i> , 1999, 302, 231-239.	2.6	40
62	Molecular structure of diatomic lanthanide compounds. <i>Science in China Series B: Chemistry</i> , 2002, 45, 91.	0.8	37
63	Relativistic theory of nuclear magnetic resonance parameters in a Gaussian basis representation. <i>Journal of Chemical Physics</i> , 2009, 131, 044129.	3.0	37
64	Spin-Multiplet Components and Energy Splittings by Multistate Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4838-4845.	4.6	37
65	Relativistic explicit correlation: Coalescence conditions and practical suggestions. <i>Journal of Chemical Physics</i> , 2012, 136, 144117.	3.0	36
66	Body-fixed relativistic molecular Hamiltonian and its application to nuclear spin-rotation tensor. <i>Journal of Chemical Physics</i> , 2013, 138, 134104.	3.0	36
67	Combining the spin-separated exact two-component relativistic Hamiltonian with the equation-of-motion coupled-cluster method for the treatment of spin-orbit splittings of light and heavy elements. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 3713-3721.	2.8	36
68	Fully relativistic theories and methods for NMR parameters. , 2012, , 187-203.		36
69	Critical Assessment of TD-DFT for Excited States of Open-Shell Systems: I. Doublet-Doublet Transitions. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 238-260.	5.3	35
70	Further development of SDSPT2 for strongly correlated electrons. <i>Molecular Physics</i> , 2017, 115, 2696-2707.	1.7	35
71	Relativistic MCSCF by means of quasidegenerate direct perturbation theory. I. Theory. <i>Journal of Chemical Physics</i> , 2000, 112, 3540-3558.	3.0	34
72	Localization of Molecular Orbitals: From Fragments to Molecule. <i>Accounts of Chemical Research</i> , 2014, 47, 2758-2767.	15.6	34

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73	On the construction of Kramers paired double group symmetry functions. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2149-2167.	2.0	33
74	Extensive theoretical studies on the low-lying electronic states of indium monochloride cation, InCl^+ . <i>Journal of Computational Chemistry</i> , 2005, 26, 106-113.	3.3	31
75	A spin-adapted size-extensive state-specific multi-reference perturbation theory with various partitioning schemes. II. Molecular applications. <i>Journal of Chemical Physics</i> , 2012, 136, 024106.	3.0	31
76	Performance of TD-DFT for Excited States of Open-Shell Transition Metal Compounds. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3929-3942.	2.5	31
77	Comprehensive theoretical studies on the low-lying electronic states of NiF , NiCl , NiBr , and NiI . <i>Journal of Chemical Physics</i> , 2006, 124, 154312.	3.0	30
78	Photoexcitation of Light-Harvesting Ca^{60} Triads: A FLMO-TD-DFT Study. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2436-2448.	5.3	30
79	Comprehensive relativistic <i>ab initio</i> and density functional theory studies on PtH , PtF , PtCl , and $\text{Pt}(\text{NH}_3)_2\text{Cl}_2$. <i>Journal of Computational Chemistry</i> , 2002, 23, 564-575.	3.3	28
80	Comment on "Four-component relativistic density functional calculations of heavy diatomic molecules" [J. Chem. Phys. 112, 3499 (2000)]. <i>Journal of Chemical Physics</i> , 2000, 113, 2506-2507.	3.0	27
81	Relativistic GWPT2 Multireference Perturbation Theory Description of the Electronic States of Y_{2} and Tc_{2} . <i>Journal of Physical Chemistry A</i> , 2014, 118, 1489-1501.	2.5	27
82	Excited states of ReO_4^- . A comprehensive time-dependent relativistic density functional theory study. <i>Chemical Physics</i> , 2009, 356, 219-228.	1.9	26
83	Perspective: Relativistic Hamiltonians. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 983-986.	2.0	26
84	Time-dependent relativistic density functional study of Yb and YbO . <i>Science in China Series B: Chemistry</i> , 2009, 52, 1945-1953.	0.8	25
85	iVI: An iterative vector interaction method for large eigenvalue problems. <i>Journal of Computational Chemistry</i> , 2017, 38, 2481-2499.	3.3	24
86	Response to "Comment on 'Quasirelativistic theory equivalent to fully relativistic theory'" [J. Chem. Phys. 123, 241102 (2005)]. <i>Journal of Chemical Physics</i> , 2006, 125, 107102.	3.0	23
87	Comprehensive <i>ab initio</i> calculation and simulation on the low-lying electronic states of TlX ($X = \text{Tl}, \text{Pb}, \text{Bi}, \text{Po}, \text{At}, \text{Rn}$). <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2436-2448.	3.3	23
88	Towards understanding the color change of 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide during gamma irradiation: an experimental and theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 18729-18735.	2.8	23
89	Further Development of iCIPT2 for Strongly Correlated Electrons. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 949-964.	5.3	23
90	Benchmark four-component relativistic density functional calculations on Cu_2 , Ag_2 , and Au_2 . <i>Chemical Physics</i> , 2005, 311, 63-69.	1.9	22

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91	Effective quantum electrodynamics hamiltonians: A tutorial review. International Journal of Quantum Chemistry, 2015, 115, 631-640.	2.0	22
92	Body-fixed relativistic molecular Hamiltonian and its application to nuclear spin-rotation tensor: Linear molecules. Journal of Chemical Physics, 2013, 139, 034113.	3.0	21
93	New Experimental NMR Shielding Scales Mapped Relativistically from NSR: Theory and Application. Journal of Chemical Theory and Computation, 2014, 10, 600-608.	5.3	21
94	Decoupling electrons and nuclei without the Born-Oppenheimer approximation: The electron-nucleus mean-field configuration-interaction method. Physical Review A, 2015, 92, .	2.5	21
95	Critical Assessment of Time-Dependent Density Functional Theory for Excited States of Open-Shell Systems: II. Doublet-Quartet Transitions. Journal of Chemical Theory and Computation, 2016, 12, 2517-2527.	5.3	21
96	NO ₂ -catalyzed deep oxidation of methanol: Experimental and theoretical studies. Journal of Molecular Catalysis A, 2006, 252, 202-211.	4.8	20
97	He@Mo ₆ Cl ₈ F ₆ : A Stable Complex of Helium. Journal of Physical Chemistry A, 2010, 114, 646-651.	2.5	20
98	Analytic Energy Gradients and Hessians of Exact Two-Component Relativistic Methods: Efficient Implementation and Extensive Applications. Journal of Chemical Theory and Computation, 2020, 16, 1541-1554.	5.3	20
99	Analytic energy gradients of spin-adapted open-shell time-dependent density functional theory. Journal of Chemical Physics, 2020, 153, 164109.	3.0	20
100	Excited states of OsO ₄ : A comprehensive time-dependent relativistic density functional theory study. Journal of Computational Chemistry, 2010, 31, 532-551.	3.3	19
101	Exact two-component relativistic energy band theory and application. Journal of Chemical Physics, 2016, 144, 044105.	3.0	19
102	Dynamic-then-Static Approach for Core Excitations of Open-Shell Molecules. Journal of Physical Chemistry Letters, 2021, 12, 7409-7417.	4.6	19
103	TD-DFT: An iterative vector interaction method for exterior/interior roots of TD-DFT. Journal of Computational Chemistry, 2019, 40, 1023-1037.	3.3	18
104	A method for population and bonding analyses in calculations with extended basis sets. Theoretica Chimica Acta, 1997, 95, 81-95.	0.8	17
105	Relativistic MCSCF by means of quasidegenerate direct perturbation theory. II. Preliminary applications. Journal of Chemical Physics, 2000, 112, 3559-3571.	3.0	17
106	SOLVATION ENERGY OF NONEQUILIBRIUM POLARIZATION: OLD QUESTION, NEW ANSWER. Journal of Theoretical and Computational Chemistry, 2010, 09, 23-37.	1.8	17
107	Relativistic Theories of NMR Shielding. , 2017, , 657-692.		17
108	iCAS: Imposed Automatic Selection and Localization of Complete Active Spaces. Journal of Chemical Theory and Computation, 2021, 17, 4846-4859.	5.3	17

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109	NAC-TDDFT: Time-Dependent Density Functional Theory for Nonadiabatic Couplings. <i>Accounts of Chemical Research</i> , 2021, 54, 3288-3297.	15.6	17
110	Theoretical study of the low-lying electronic excited states for molecular aggregates. <i>Science China Chemistry</i> , 2013, 56, 1258-1262.	8.2	16
111	Localization of open-shell molecular orbitals via least change from fragments to molecule. <i>Journal of Chemical Physics</i> , 2017, 146, 104104.	3.0	16
112	Role of Planar Conformations in Aggregation Induced Spectral Shifts of Supermolecular Oligofluorenes in Solutions and Films: A Combined Experimental and MD/TD-DFT Study. <i>Journal of Physical Chemistry B</i> , 2015, 119, 10316-10333.	2.6	15
113	iCISCF: An Iterative Configuration Interaction-Based Multiconfigurational Self-Consistent Field Theory for Large Active Spaces. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7545-7561.	5.3	15
114	Orbital localization and delocalization effects in the U5f2 configuration: Impurity problem. <i>Physical Review B</i> , 1998, 57, 10648-10654.	3.2	13
115	Theoretical study on the low-lying electronic states of NiH and NiAt. <i>Journal of Computational Chemistry</i> , 2007, 28, 2286-2298.	3.3	13
116	Towards Near-Infrared Chiroptically Switching Materials: Theoretical and Experimental Studies on Viologen-Containing 1,1'-Binaphthyls. <i>ChemPhysChem</i> , 2008, 9, 1265-1269.	2.1	13
117	The Static-Dynamic-Static Family of Methods for Strongly Correlated Electrons: Methodology and Benchmarking. <i>Topics in Current Chemistry</i> , 2021, 379, 43.	5.8	13
118	On Relativity, Bonding, and Valence Electron Distribution. <i>Journal of Physical Chemistry A</i> , 2002, 106, 795-803.	2.5	10
119	A quantum chemical definition of electron-nucleus correlation. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	1.4	10
120	SOiCI and iCISO: combining iterative configuration interaction with spin-orbit coupling in two ways. <i>Journal of Physics Condensed Matter</i> , 2022, 34, 224007.	1.8	10
121	The 'big picture' of relativistic molecular quantum mechanics. <i>AIP Conference Proceedings</i> , 2012, , .	0.4	9
122	No-Pair Relativistic Hamiltonians: Q4C and X2C. , 2017, , 375-393.		9
123	Relativistic theory of nuclear spin-rotation tensor with kinetically balanced rotational London orbitals. <i>Journal of Chemical Physics</i> , 2014, 141, 164110.	3.0	8
124	Relativistic quantum chemistry: today and tomorrow. <i>Scientia Sinica Chimica</i> , 2020, 50, 1672-1696.	0.4	8
125	On the performance of the open-shell perturbation theory. <i>Science China Chemistry</i> , 2011, 54, 446-453.	8.2	7
126	With-Pair Relativistic Hamiltonians. , 2017, , 345-373.		7

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127	iOI: An Iterative Orbital Interaction Approach for Solving the Self-Consistent Field Problem. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4831-4845.	5.3	7
128	Publisher's Note: "Four-component relativistic theory for NMR parameters: Unified formulation and numerical assessment of different approaches" [<i>J. Chem. Phys.</i> 130, 144102 (2009)]. <i>Journal of Chemical Physics</i> , 2009, 131, 019902.	3.0	6
129	Spin Separation of Relativistic Hamiltonians. , 2017, , 411-447.		6
130	Matrix formulation of direct perturbation theory of relativistic effects in a kinetically balanced basis. <i>Chemical Physics</i> , 2008, 349, 133-146.	1.9	5
131	Basic Structures of Relativistic Wave Functions. , 2017, , 481-496.		5
132	Tuning mesomorphic properties and handedness of chiral calamitic liquid crystals by minimal modification of the effective core. <i>Chirality</i> , 2011, 23, E74-83.	2.6	4
133	Theoretical study of low-lying excited states of molecular aggregates. I. Development of linear-scaling TD-DFT. <i>Science China Chemistry</i> , 2013, 56, 1263-1266.	8.2	4
134	Relativistic Explicit Correlation: Problems and Solutions. , 2017, , 531-545.		4
135	Electronic coupling matrix elements of U-shaped donor-bridge-acceptor molecules and influence of mediated benzene solvent. <i>Chemical Physics Letters</i> , 2005, 414, 71-75.	2.6	3
136	Ab initio investigation on electron transfer in molecular electronic devices: A minimal model study. <i>Chemical Physics Letters</i> , 2007, 439, 85-90.	2.6	3
137	Effective quantum electrodynamics hamiltonians: A tutorial review. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 971-971.	2.0	3
138	Electronic transitions of tantalum monofluoride. <i>Journal of Chemical Physics</i> , 2017, 146, 094308.	3.0	2
139	Relativistic Theory of Nuclear Spin-Rotation Tensor. , 2017, , 693-723.		2
140	Coalescence Conditions of Relativistic Wave Functions. , 2017, , 497-530.		2
141	Relativistic Theories of NMR Shielding. , 2015, , 1-33.		2
142	With-Pair Relativistic Hamiltonians. , 2014, , 1-26.		2
143	Tuning Catalyst-Free Photocontrolled Polymerization by Substitution: A Quantitative and Qualitative Interpretation. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 3290-3296.	4.6	2
144	Special issue of <i>Chemical Physics</i> on recent advances and applications of relativistic quantum chemistry. <i>Chemical Physics</i> , 2012, 395, 1.	1.9	1

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145	Sublinear scaling quantum chemical methods for magnetic shieldings in large molecules. Journal of Chemical Physics, 2019, 150, 154113.	3.0	1
146	Basic Structures of Relativistic Wave Functions. , 2015, , 1-14.		1
147	Quasirelativistic theory. , 2006, , 909-910.		1
148	With-Pair Relativistic Hamiltonians. , 2016, , 1-29.		1
149	Relativistic Explicit Correlation: Problems and Solutions. , 2015, , 1-13.		0
150	A novel infinite-order quasirelativistic density functional theory. , 2006, , 919-922.		0
151	With-Pair Relativistic Hamiltonians. , 2015, , 1-29.		0
152	Coalescence Conditions of Relativistic Wave Functions. , 2015, , 1-31.		0
153	No-Pair Relativistic Hamiltonians: Q4C and X2C. , 2015, , 1-17.		0
154	Relativistic Theory of Nuclear Spin-Rotation Tensor. , 2015, , 1-31.		0
155	Spin Separation of Relativistic Hamiltonians. , 2015, , 1-33.		0