Wenjian Liu

List of Publications by Citations

154 papers	5,969 citations	47 h-index	71 g-index
166 ext. papers	6,697 ext. citations	5.4 avg, IF	6.45 L-index

#	Paper	IF	Citations
154	Quasirelativistic theory equivalent to fully relativistic theory. *Journal of Chemical Physics*, **2005**, 123, 241102	3.9	316
153	Ideas of relativistic quantum chemistry. *Molecular Physics*, **2010**, 108, 1679-1706	1.7	242
152	Exact two-component Hamiltonians revisited. *Journal of Chemical Physics*, **2009**, 131, 031104	3.9	221
151	The Beijing four-component density functional program package (BDF) and its application to EuO, EuS, YbO and YbS. *Theoretical Chemistry Accounts*, **1997**, 96, 75-83	1.9	201
150	Infinite-order quasirelativistic density functional method based on the exact matrix quasirelativistic theory. *Journal of Chemical Physics*, **2006**, 125, 44102	3.9	186
149	Making four- and two-component relativistic density functional methods fully equivalent based on the idea of "from atoms to molecule". *Journal of Chemical Physics*, **2007**, 127, 104106	3.9	175
148	Quasirelativistic theory. II. Theory at matrix level. *Journal of Chemical Physics*, **2007**, 126, 114107	3.9	126
147	A small-core multiconfiguration Dirac–Hartree–Fock-adjusted pseudopotential for Tl application to TlX (X = F, Cl, Br, I). *Theoretical Chemistry Accounts*, **2000**, 104, 22-28	1.9	122
146	Morphological effects of the nanostructured ceria support on the activity and stability of CuO/CeO2 catalysts for the water-gas shift reaction. *Physical Chemistry Chemical Physics*, **2014**, 16, 17183-95	3.6	120
145	The Beijing Density Functional (BDF) Program Package: Methodologies and Applications. *Journal of Theoretical and Computational Chemistry*, **2003**, 02, 257-272	1.8	114
144	Unraveling the Dynamic Nature of a CuO/CeO2 Catalyst for CO Oxidation in Operando: A Combined Study of XANES (Fluorescence) and DRIFTS. *ACS Catalysis*, **2014**, 4, 1650-1661	13.1	106
143	Advances in relativistic molecular quantum mechanics. *Physics Reports*, **2014**, 537, 59-89	27.7	99
142	On the spin separation of algebraic two-component relativistic Hamiltonians. *Journal of Chemical Physics*, **2012**, 137, 154114	3.9	97
141	Quasirelativistic theory I. Theory in terms of a quasi-relativistic operator. *Molecular Physics*, **2006**, 104, 2225-2240	1.7	96
140	Spectroscopic constants of gold and eka-gold (element 111) diatomic compounds: The importance of spin–orbit coupling. *Journal of Chemical Physics*, **1999**, 110, 3730-3735	3.9	92
139	iCI: Iterative CI toward full CI. *Journal of Chemical Theory and Computation*, **2016**, 12, 1169-78	6.4	90
138	Time-dependent four-component relativistic density functional theory for excitation energies. *Journal of Chemical Physics*, **2004**, 121, 6658-66	3.9	85

137	Time-dependent four-component relativistic density-functional theory for excitation energies. II. The exchange-correlation kernel. *Journal of Chemical Physics*, **2005**, 123, 054102	3.9	80
136	Four-component relativistic theory for nuclear magnetic shielding constants: critical assessments of different approaches. *Journal of Chemical Physics*, **2007**, 126, 214101	3.9	70
135	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). *International Journal of Quantum Chemistry*, **2000**, 76, 359-370	2.1	70
134	Combining spin-adapted open-shell TD-DFT with spin–orbit coupling. *Molecular Physics*, **2013**, 111, 3741-3755	1.7	69
133	Ab initio pseudopotential and density-functional all-electron study of ionization and excitation energies of actinide atoms. *Physical Review A*, **1998**, 58, 1103-1110	2.6	68
132	Comparison of Different Polarization Schemes in Open-shell Relativistic Density Functional Calculations. *Journal of the Chinese Chemical Society*, **2003**, 50, 597-606	1.5	66
131	Fully relativistic density functional calculations of the ground and excited states of Yb, YbH, YbF, and YbO. *Journal of Chemical Physics*, **1998**, 108, 2886-2895	3.9	65
130	Four-component relativistic theory for nuclear magnetic shielding: magnetically balanced gauge-including atomic orbitals. *Journal of Chemical Physics*, **2009**, 131, 244113	3.9	64
129	Computer-Guided Discovery of a pH-Responsive Organic Photocatalyst and Application for pH and Light Dual-Gated Polymerization. *Journal of the American Chemical Society*, **2019**, 141, 8207-8220	16.4	63
128	Perspectives of relativistic quantum chemistry: the negative energy cat smiles. *Physical Chemistry Chemical Physics*, **2012**, 14, 35-48	3.6	62
127	Low-lying electronic states of lanthanocenes and actinocenes M(C8H8)2 (M=Nd, Tb, Yb, U). *Journal of Chemical Physics*, **1997**, 107, 3584-3591	3.9	62
126	Spin-adapted open-shell time-dependent density functional theory. II. Theory and pilot application. *Journal of Chemical Physics*, **2011**, 134, 134101	3.9	60
125	Spin-adapted open-shell random phase approximation and time-dependent density functional theory. I. Theory. *Journal of Chemical Physics*, **2010**, 133, 064106	3.9	60
124	First-order nonadiabatic coupling matrix elements between excited states: a Lagrangian formulation at the CIS, RPA, TD-HF, and TD-DFT levels. *Journal of Chemical Physics*, **2014**, 141, 014110	3.9	59
123	First order nonadiabatic coupling matrix elements between excited states: implementation and application at the TD-DFT and pp-TDA levels. *Journal of Chemical Physics*, **2014**, 141, 244105	3.9	59
122	Linear-Scaling Time-Dependent Density Functional Theory Based on the Idea of "From Fragments to Molecule". *Journal of Chemical Theory and Computation*, **2011**, 7, 3643-60	6.4	58
121	Time-dependent quasirelativistic density-functional theory based on the zeroth-order regular approximation. *Journal of Chemical Physics*, **2005**, 123, 144101	3.9	58
120	Spectroscopic constants of Pb and Eka-lead compounds: comparison of different approaches. *Advances in Quantum Chemistry*, **2001**, 325-355	1.4	57

119	Theoretical and numerical assessments of spin-flip time-dependent density functional theory. *Journal of Chemical Physics*, **2012**, 136, 024107	3.9	56
118	Solvent effects on the optical spectra and excited-state decay of triphenylamine-thiadiazole with hybridized local excitation and intramolecular charge transfer. *Journal of Physical Chemistry A*, **2015**, 119, 5233-40	2.8	55
117	Comparison of restricted, unrestricted, inverse, and dual kinetic balances for four-component relativistic calculations. *Theoretical Chemistry Accounts*, **2011**, 129, 423-436	1.9	55
116	Four-component relativistic theory for NMR parameters: unified formulation and numerical assessment of different approaches. *Journal of Chemical Physics*, **2009**, 130, 144102	3.9	55
115	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. *Journal of Chemical Physics*, **2002**, 116, 3626-3634	3.9	55
114	Four-component relativistic theory for nuclear magnetic shielding constants: the orbital decomposition approach. *Journal of Chemical Physics*, **2007**, 126, 081101	3.9	54
113	Benchmark calculations for lanthanide atoms: Calibration of ab initio and density-functional methods. *Physical Review A*, **1998**, 57, 1721-1728	2.6	53
112	Going beyond "no-pair relativistic quantum chemistry". *Journal of Chemical Physics*, **2013**, 139, 014108	3.9	52
111	The Ground State Electronic Energy of Benzene. *Journal of Physical Chemistry Letters*, **2020**, 11, 8922-8929	6.4	52
110	On the spin separation of algebraic two-component relativistic Hamiltonians: molecular properties. *Journal of Chemical Physics*, **2014**, 141, 054111	3.9	50
109	Spin-adapted open-shell time-dependent density functional theory. III. An even better and simpler formulation. *Journal of Chemical Physics*, **2011**, 135, 194106	3.9	49
108	Exact two-component relativistic theory for nuclear magnetic resonance parameters. *Journal of Chemical Physics*, **2009**, 131, 081101	3.9	49
107	Exact two-component relativistic theory for NMR parameters: general formulation and pilot application. *Journal of Chemical Physics*, **2012**, 137, 174105	3.9	47
106	SDS: the Static Dynamic Static framework for strongly correlated electrons. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	46
105	A spin-adapted size-extensive state-specific multi-reference perturbation theory. I. Formal developments. *Journal of Chemical Physics*, **2012**, 136, 024105	3.9	42
104	Calculated Properties of Lanthanocene Anions and the Unusual Electronic Structure of Their Neutral Counterparts. *Inorganic Chemistry*, **1998**, 37, 1067-1072	5.1	42
103	Big picture of relativistic molecular quantum mechanics. *National Science Review*, **2016**, 3, 204-221	10.8	41
102	Fully relativistic theories and methods for NMR parameters. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	41

101	RELATIVISTIC DENSITY FUNCTIONAL THEORY: THE BDF PROGRAM PACKAGE. *Recent Advances in Computational*, **2004**, 257-282		39
100	Relativistic time-dependent density functional theories. *Chemical Society Reviews*, **2018**, 47, 4481-4509	58.5	37
99	Relativistic ab initio and density functional theory calculations on the mercury fluorides: Is HgF4 thermodynamically stable?. *Chemical Physics Letters*, **1999**, 302, 231-239	2.5	36
98	Body-fixed relativistic molecular Hamiltonian and its application to nuclear spin-rotation tensor. *Journal of Chemical Physics*, **2013**, 138, 134104	3.9	35
97	Iterative Configuration Interaction with Selection. *Journal of Chemical Theory and Computation*, **2020**, 16, 2296-2316	6.4	34
96	Molecular structure of diatomic lanthanide compounds. *Science in China Series B: Chemistry*, **2002**, 45, 91		34
95	Relativistic explicit correlation: coalescence conditions and practical suggestions. *Journal of Chemical Physics*, **2012**, 136, 144117	3.9	31
94	A spin-adapted size-extensive state-specific multi-reference perturbation theory with various partitioning schemes. II. Molecular applications. *Journal of Chemical Physics*, **2012**, 136, 024106	3.9	31
93	Relativistic MCSCF by means of quasidegenerate direct perturbation theory. I. Theory. *Journal of Chemical Physics*, **2000**, 112, 3540-3558	3.9	31
92	Relativistic theory of nuclear magnetic resonance parameters in a Gaussian basis representation. *Journal of Chemical Physics*, **2009**, 131, 044129	3.9	30
91	Comprehensive theoretical studies on the low-lying electronic states of NiF, NiCl, NiBr, and NiI. *Journal of Chemical Physics*, **2006**, 124, 154312	3.9	30
90	On the construction of Kramers paired double group symmetry functions. *International Journal of Quantum Chemistry*, **2009**, 109, 2149-2167	2.1	29
89	Extensive theoretical studies on the low-lying electronic states of indium monochloride cation, InCl+. *Journal of Computational Chemistry*, **2005**, 26, 106-13	3.5	29
88	BDF: A relativistic electronic structure program package. *Journal of Chemical Physics*, **2020**, 152, 064113	3.9	28
87	Critical Assessment of TD-DFT for Excited States of Open-Shell Systems: I. Doublet-Doublet Transitions. *Journal of Chemical Theory and Computation*, **2016**, 12, 238-60	6.4	28
86	Localization of molecular orbitals: from fragments to molecule. *Accounts of Chemical Research*, **2014**, 47, 2758-67	24.3	28
85	Photoexcitation of Light-Harvesting C-P-C60 Triads: A FLMO-TD-DFT Study. *Journal of Chemical Theory and Computation*, **2014**, 10, 2436-48	6.4	28
84	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. *Physical Chemistry Chemical Physics*, **2017**, 19, 3713-3721	3.6	26

83	Further development of SDSPT2 for strongly correlated electrons. *Molecular Physics*, **2017**, 115, 2696-2707	1.7	26
82	Comprehensive relativistic ab initio and density functional theory studies on PtH, PtF, PtCl, and Pt(NH(3))(2)Cl(2). *Journal of Computational Chemistry*, **2002**, 23, 564-75	3.5	25
81	Comment on Four-component relativistic density functional calculations of heavy diatomic molecules[J. Chem. Phys. 112, 3499 (2000)]. *Journal of Chemical Physics*, **2000**, 113, 2506-2507	3.9	25
80	Excited states of ReO4-: A comprehensive time-dependent relativistic density functional theory study. *Chemical Physics*, **2009**, 356, 219-228	2.3	24
79	Relativistic GVVPT2 multireference perturbation theory description of the electronic states of Y2 and Tc2. *Journal of Physical Chemistry A*, **2014**, 118, 1489-501	2.8	23
78	Spin-Multiplet Components and Energy Splittings by Multistate Density Functional Theory. *Journal of Physical Chemistry Letters*, **2017**, 8, 4838-4845	6.4	23
77	Time-dependent relativistic density functional study of Yb and YbO. *Science in China Series B: Chemistry*, **2009**, 52, 1945-1953		23
76	Essentials of relativistic quantum chemistry. *Journal of Chemical Physics*, **2020**, 152, 180901	3.9	22
75	Body-fixed relativistic molecular Hamiltonian and its application to nuclear spin-rotation tensor: linear molecules. *Journal of Chemical Physics*, **2013**, 139, 034113	3.9	21
74	Benchmark four-component relativistic density functional calculations on Cu2, Ag2, and Au2. *Chemical Physics*, **2005**, 311, 63-69	2.3	21
73	Performance of TD-DFT for Excited States of Open-Shell Transition Metal Compounds. *Journal of Physical Chemistry A*, **2017**, 121, 3929-3942	2.8	20
72	New Experimental NMR Shielding Scales Mapped Relativistically from NSR: Theory and Application. *Journal of Chemical Theory and Computation*, **2014**, 10, 600-8	6.4	20
71	Response to Comment on Quasirelativistic theory equivalent to fully relativistic theory[J. Chem. Phys. 123, 241102 (2005)]. *Journal of Chemical Physics*, **2006**, 125, 107102	3.9	20
70	Unravelling an oxygen-mediated reductive quenching pathway for photopolymerisation under long wavelengths. *Nature Communications*, **2021**, 12, 478	17.4	20
69	Towards understanding the color change of 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide during gamma irradiation: an experimental and theoretical study. *Physical Chemistry Chemical Physics*, **2014**, 16, 18729-35	3.6	19
68	Perspective: Relativistic Hamiltonians. *International Journal of Quantum Chemistry*, **2014**, 114, 983-986	2.1	19
67	Excited states of OsO4: a comprehensive time-dependent relativistic density functional theory study. *Journal of Computational Chemistry*, **2010**, 31, 532-51	3.5	18
66	SOLVATION ENERGY OF NONEQUILIBRIUM POLARIZATION: OLD QUESTION, NEW ANSWER. *Journal of Theoretical and Computational Chemistry*, **2010**, 09, 23-37	1.8	17

65	He@Mo(6)Cl(8)F(6): a stable complex of helium. *Journal of Physical Chemistry A*, **2010**, 114, 646-51	2.8	17
64	A method for population and bonding analyses in calculations with extended basis sets. *Theoretica Chimica Acta*, **1997**, 95, 81-95		17
63	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, 2517-27	6.4	17
62	iVI: An iterative vector interaction method for large eigenvalue problems. *Journal of Computational Chemistry*, **2017**, 38, 2481-2499	3.5	16
61	Comprehensive ab initio calculation and simulation on the low-lying electronic states of TlX (X = F, Cl, Br, I, and At). *Journal of Computational Chemistry*, **2009**, 30, 524-39	3.5	16
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58	Effective quantum electrodynamics hamiltonians: A tutorial review. *International Journal of Quantum Chemistry*, **2015**, 115, 631-640	2.1	15
57	Theoretical study of the low-lying electronic excited states for molecular aggregates. *Science China Chemistry*, **2013**, 56, 1258-1262	7.9	15
56	Role of Planar Conformations in Aggregation Induced Spectral Shifts of Supermolecular Oligofluorenols in Solutions and Films: A Combined Experimental and MD/TD-DFT Study. *Journal of Physical Chemistry B*, **2015**, 119, 10316-33	3.4	14
55	Decoupling electrons and nuclei without the Born-Oppenheimer approximation: The electron-nucleus mean-field configuration-interaction method. *Physical Review A*, **2015**, 92,	2.6	14
54	Rational Design of Photocatalysts for Controlled Polymerization: Effect of Structures on Photocatalytic Activities.. *Chemical Reviews*, **2022**,	68.1	14
53	Exact two-component relativistic energy band theory and application. *Journal of Chemical Physics*, **2016**, 144, 044105	3.9	14
52	Theoretical study on the low-lying electronic states of NiH and NiAt. *Journal of Computational Chemistry*, **2007**, 28, 2286-98	3.5	13
51	Localization of open-shell molecular orbitals via least change from fragments to molecule. *Journal of Chemical Physics*, **2017**, 146, 104104	3.9	12
50	Towards near-infrared chiroptically switching materials: theoretical and experimental studies on viologen-containing 1,1'-binaphthyls. *ChemPhysChem*, **2008**, 9, 1265-9	3.2	12
49	Recent Advances in Relativistic Density Functional Methods		12
48	iVI-TD-DFT: An iterative vector interaction method for exterior/interior roots of TD-DFT. *Journal of Computational Chemistry*, **2019**, 40, 1023-1037	3.5	11

47	Orbital localization and delocalization effects in the U 5f2 configuration: Impurity problem. *Physical Review B*, **1998**, 57, 10648-10654	3.3	10
46	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	6.4	10
45	Relativistic Theories of NMR Shielding **2017**, 657-692		9
44	The 'big picture' of relativistic molecular quantum mechanics **2012**,		9
43	On Relativity, Bonding, and Valence Electron Distribution. *Journal of Physical Chemistry A*, **2002**, 106, 795-803	2.8	9
42	Analytic energy gradients of spin-adapted open-shell time-dependent density functional theory. *Journal of Chemical Physics*, **2020**, 153, 164109	3.9	9
41	A quantum chemical definition of electron□nucleus correlation. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	8
40	Relativistic theory of nuclear spin-rotation tensor with kinetically balanced rotational London orbitals. *Journal of Chemical Physics*, **2014**, 141, 164110	3.9	8
39	iCAS: Imposed Automatic Selection and Localization of Complete Active Spaces. *Journal of Chemical Theory and Computation*, **2021**, 17, 4846-4859	6.4	7
38	Further Development of iCIPT2 for Strongly Correlated Electrons. *Journal of Chemical Theory and Computation*, **2021**, 17, 949-964	6.4	7
37	No-Pair Relativistic Hamiltonians:Q4C and X2C **2017**, 375-393		6
36	On the performance of the open-shell perturbation theory. *Science China Chemistry*, **2011**, 54, 446-453	7.9	6
35	Publisher's Note: "Four-component relativistic theory for NMR parameters: unified formulation and numerical assessment of different approaches" [J. Chem. Phys. 130, 144102 (2009)]. *Journal of Chemical Physics*, **2009**, 131, 019902	3.9	5
34	Matrix formulation of direct perturbation theory of relativistic effects in a kinetically balanced basis. *Chemical Physics*, **2008**, 349, 133-146	2.3	5
33	iCISCF: An Iterative Configuration Interaction-Based Multiconfigurational Self-Consistent Field Theory for Large Active Spaces. *Journal of Chemical Theory and Computation*, **2021**,	6.4	5
32	Dynamic-then-Static Approach for Core Excitations of Open-Shell Molecules. *Journal of Physical Chemistry Letters*, **2021**, 12, 7409-7417	6.4	5
31	Theoretical study of low-lying excited states of molecular aggregates. I. Development of linear-scaling TD-DFT. *Science China Chemistry*, **2013**, 56, 1263-1266	7.9	4
30	Tuning mesomorphic properties and handedness of chiral calamitic liquid crystals by minimal modification of the effective core. *Chirality*, **2011**, 23 Suppl 1, E74-83	2.1	4

29	Relativistic quantum chemistry: today and tomorrow. *Scientia Sinica Chimica*, **2020**, 50, 1672-1696	1.6	4
28	iOI: An Iterative Orbital Interaction Approach for Solving the Self-Consistent Field Problem. *Journal of Chemical Theory and Computation*, **2021**, 17, 4831-4845	6.4	4
27	Spin Separation of Relativistic Hamiltonians **2017**, 411-447		3
26	Basic Structures of RelativisticWave Functions **2017**, 481-496		3
25	Relativistic Explicit Correlation: Problemsand Solutions **2017**, 531-545		3
24	Ab initio investigation on electron transfer in molecular electronic devices: A minimal model study. *Chemical Physics Letters*, **2007**, 439, 85-90	2.5	3
23	Electronic coupling matrix elements of U-shaped donor-bridge-acceptor molecules and influence of mediated benzene solvent. *Chemical Physics Letters*, **2005**, 414, 71-75	2.5	3
22	NAC-TDDFT: Time-Dependent Density Functional Theory for Nonadiabatic Couplings. *Accounts of Chemical Research*, **2021**, 54, 3288-3297	24.3	3
21	Electronic transitions of tantalum monofluoride. *Journal of Chemical Physics*, **2017**, 146, 094308	3.9	2
20	With-Pair Relativistic Hamiltonians **2017**, 345-373		2
19	Relativistic Theory of Nuclear Spin-Rotation Tensor **2017**, 693-723		2
18	Coalescence Conditions of Relativistic Wave Functions **2017**, 497-530		2
17	The Static-Dynamic-Static Family of Methods for Strongly Correlated Electrons: Methodology and Benchmarking. *Topics in Current Chemistry*, **2021**, 379, 43	7.2	2
16	Fully relativistic theories and methods for NMR parameters **2012**, 187-203		2
15	Relativistic Theories of NMR Shielding **2015**, 1-33		2
14	Sublinear scaling quantum chemical methods for magnetic shieldings in large molecules. *Journal of Chemical Physics*, **2019**, 150, 154113	3.9	1
13	Quasirelativistic theory **2006**, 909-910		1
12	Basic Structures of Relativistic Wave Functions **2015**, 1-14		1

11	Tuning Catalyst-Free Photocontrolled Polymerization by Substitution: A Quantitative and Qualitative Interpretation.. *Journal of Physical Chemistry Letters*, **2022**, 3290-3296	6.4	0
10	Relativistic Explicit Correlation: Problems and Solutions **2015**, 1-13		
9	A novel infinite-order quasirelativistic density functional theory **2006**, 919-922		
8	With-Pair Relativistic Hamiltonians **2015**, 1-29		
7	Coalescence Conditions of Relativistic Wave Functions **2015**, 1-31		
6	No-Pair Relativistic Hamiltonians: Q4C and X2C **2015**, 1-17		
5	Relativistic Theory of Nuclear Spin-Rotation Tensor **2015**, 1-31		
4	Spin Separation of Relativistic Hamiltonians **2015**, 1-33		
3	With-Pair Relativistic Hamiltonians **2016**, 1-29		
2	With-Pair Relativistic Hamiltonians **2014**, 1-26		
1	The Static-Dynamic-Static Family of Methods for Strongly Correlated Electrons: Methodology and Benchmarking. *Topics in Current Chemistry Collections*, **2022**, 181-236	1.8	