Wenjian Liu

List of Publications by Year
in descending order

155 papers	7,569 citations	31976 53 h-index	60623 81 g-index
166 all docs	166 docs citations	166 times ranked	3354 citing authors

#	Article	IF	Citations
1	Rational Design of Photocatalysts for Controlled Polymerization: Effect of Structures on Photocatalytic Activities. Chemical Reviews, 2022, 122, 5476-5518.	47.7	106
2	Tuning Catalyst-Free Photocontrolled Polymerization by Substitution: A Quantitative and Qualitative Interpretation. Journal of Physical Chemistry Letters, 2022, 13, 3290-3296.	4.6	2
3	SOiCI and iCISO: combining iterative configuration interaction with spinâ€“orbit coupling in two ways. Journal of Physics Condensed Matter, 2022, 34, 224007.	1.8	10
4	Further Development of iCIPT2 for Strongly Correlated Electrons. Journal of Chemical Theory and Computation, 2021, 17, 949-964.	5.3	23
5	Dynamic-then-Static Approach for Core Excitations of Open-Shell Molecules. Journal of Physical Chemistry Letters, 2021, 12, 7409-7417.	4.6	19
6	iCAS: Imposed Automatic Selection and Localization of Complete Active Spaces. Journal of Chemical Theory and Computation, 2021, 17, 4846-4859.	5.3	17
7	iOI: An Iterative Orbital Interaction Approach for Solving the Self-Consistent Field Problem. Journal of Chemical Theory and Computation, 2021, 17, 4831-4845.	5.3	7
8	NAC-TDDFT: Time-Dependent Density Functional Theory for Nonadiabatic Couplings. Accounts of Chemical Research, 2021, 54, 3288-3297.	15.6	17
9	Unravelling an oxygen-mediated reductive quenching pathway for photopolymerisation under long wavelengths. Nature Communications, 2021, 12, 478.	12.8	54
10	The Staticâ€“Dynamicâ€“Static Family of Methods for Strongly Correlated Electrons: Methodology and Benchmarking. Topics in Current Chemistry, 2021, 379, 43.	5.8	13
11	iCISCF: An Iterative Configuration Interaction-Based Multiconfigurational Self-Consistent Field Theory for Large Active Spaces. Journal of Chemical Theory and Computation, 2021, 17, 7545-7561.	5.3	15
12	The Ground State Electronic Energy of Benzene. Journal of Physical Chemistry Letters, 2020, 11, 8922-8929.	4.6	90
13	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
14	Analytic energy gradients of spin-adapted open-shell time-dependent density functional theory. Journal of Chemical Physics, 2020, 153, 164109.	3.0	20
15	Essentials of relativistic quantum chemistry. Journal of Chemical Physics, 2020, 152, 180901.	3.0	57
16	BDF: A relativistic electronic structure program package. Journal of Chemical Physics, 2020, 152, 064113.	3.0	79
17	Iterative Configuration Interaction with Selection. Journal of Chemical Theory and Computation, 2020, 16, 2296-2316.	5.3	67
18	Relativistic quantum chemistry: today and tomorrow. Scientia Sinica Chimica, 2020, 50, 1672-1696.	0.4	8

#	Article	IF	Citations
19	Sublinear scaling quantum chemical methods for magnetic shieldings in large molecules. Journal of Chemical Physics, 2019, 150, 154113.	3.0	1
20	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.	13.7	89
21	iVIâ€TDâ€DFT: An iterative vector interaction method for exterior/interior roots of TDâ€DFT. Journal of Computational Chemistry, 2019, 40, 1023-1037.	3.3	18
22	Relativistic time-dependent density functional theories. Chemical Society Reviews, 2018, 47, 4481-4509.	38.1	54
23	Combining the spin-separated exact two-component relativistic Hamiltonian with the equation-of-motion coupled-cluster method for the treatment of spinâ€“orbit splittings of light and heavy elements. Physical Chemistry Chemical Physics, 2017, 19, 3713-3721.	2.8	36
24	A quantum chemical definition of electronâ€“nucleus correlation. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	10
25	Electronic transitions of tantalum monofluoride. Journal of Chemical Physics, 2017, 146, 094308.	3.0	2
26	Localization of open-shell molecular orbitals via least change from fragments to molecule. Journal of Chemical Physics, 2017, 146, 104104.	3.0	16
27	Further development of SDSPT2 for strongly correlated electrons. Molecular Physics, 2017, 115, 2696-2707.	1.7	35
28	Performance of TD-DFT for Excited States of Open-Shell Transition Metal Compounds. Journal of Physical Chemistry A, 2017, 121, 3929-3942.	2.5	31
29	Spin-Multiplet Components and Energy Splittings by Multistate Density Functional Theory. Journal of Physical Chemistry Letters, 2017, 8, 4838-4845.	4.6	37
30	iVI: An iterative vector interaction method for large eigenvalue problems. Journal of Computational Chemistry, 2017, 38, 2481-2499.	3.3	24
31	With-Pair Relativistic Hamiltonians. , 2017, , 345-373.		7
32	Relativistic Theory of Nuclear Spin-Rotation Tensor. , 2017, , 693-723.		2
33	Relativistic Theories of NMR Shielding. , 2017, , 657-692.		17
34	No-Pair Relativistic Hamiltonians:Q4C and X2C. , 2017, , 375-393.		9
35	Spin Separation of Relativistic Hamiltonians. , 2017, , 411-447.		6
36	Basic Structures of RelativisticWave Functions. , 2017, , 481-496.		5

#	Article	IF	Citations
37	Coalescence Conditions of Relativistic Wave Functions. , 2017, , 497-530.		2
38	Relativistic Explicit Correlation: Problemsand Solutions. , 2017, , 531-545.		4
39	Exact two-component relativistic energy band theory and application. Journal of Chemical Physics, 2016, 144, 044105.	3.0	19
40	Effective quantum electrodynamics hamiltonians: A tutorial review. International Journal of Quantum Chemistry, 2016, 116, 971-971.	2.0	3
41	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
42	iCI: Iterative CI toward full CI. Journal of Chemical Theory and Computation, 2016, 12, 1169-1178.	5.3	123
43	Big picture of relativistic molecular quantum mechanics. National Science Review, 2016, 3, 204-221.	9.5	54
44	Critical Assessment of TD-DFT for Excited States of Open-Shell Systems: I. Doubletâ€“Doublet Transitions. Journal of Chemical Theory and Computation, 2016, 12, 238-260.	5.3	35
45	With-Pair Relativistic Hamiltonians. , 2016, , 1-29.		1
46	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
47	Effective quantum electrodynamics hamiltonians: A tutorial review. International Journal of Quantum Chemistry, 2015, 115, 631-640.	2.0	22
48	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, 10316-10333.	2.6	15
49	Relativistic Explicit Correlation: Problems and Solutions. , 2015, , 1-13.		0
50	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, 5233-5240.	2.5	73
51	Relativistic Theories of NMR Shielding. , 2015, , 1-33.		2
52	Basic Structures of Relativistic Wave Functions. , 2015, , 1-14.		1
53	With-Pair Relativistic Hamiltonians. , 2015, , 1-29.		0
54	Coalescence Conditions of Relativistic Wave Functions. , 2015, , 1-31.		0

#	Article	IF	Citations
55	No-Pair Relativistic Hamiltonians: Q4C and X2C. , 2015, , 1-17.		0
56	Relativistic Theory of Nuclear Spin-Rotation Tensor. , 2015, , 1-31.		0
57	Spin Separation of Relativistic Hamiltonians. , 2015, , 1-33.		0
58	Relativistic theory of nuclear spin-rotation tensor with kinetically balanced rotational London orbitals. Journal of Chemical Physics, 2014, 141, 164110.	3.0	8
59	On the spin separation of algebraic two-component relativistic Hamiltonians: Molecular properties. Journal of Chemical Physics, 2014, 141, 054111.	3.0	67
60	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.	3.0	74
61	SDS: the â€˜staticâ€“dynamicâ€“staticâ€™ framework for strongly correlated electrons. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	61
62	Advances in relativistic molecular quantum mechanics. Physics Reports, 2014, 537, 59-89.	25.6	122
63	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, 18729-18735.	2.8	23
64	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, 17183-17195.	2.8	143
65	Localization of Molecular Orbitals: From Fragments to Molecule. Accounts of Chemical Research, 2014, 47, 2758-2767.	15.6	34
66	Relativistic GVVPT2 Multireference Perturbation Theory Description of the Electronic States of Y₂ and Tc₂. Journal of Physical Chemistry A, 2014, 118, 1489-1501.	2.5	27
67	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
68	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.	3.0	83
69	Photoexcitation of Light-Harvesting Câ€“Pâ€“C₆₀ Triads: A FLMO-TD-DFT Study. Journal of Chemical Theory and Computation, 2014, 10, 2436-2448.	5.3	30
70	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.	11.2	128
71	Perspective: Relativistic Hamiltonians. International Journal of Quantum Chemistry, 2014, 114, 983-986.	2.0	26
72	With-Pair Relativistic Hamiltonians. , 2014, , 1-26.		2

#	Article	IF	Citations
73	Theoretical study of the low-lying electronic excited states for molecular aggregates. Science China Chemistry, 2013, 56, 1258-1262.	8.2	16
74	Theoretical study of low-lying excited states of molecular aggregates. I. Development of linear-scaling TD-DFT. Science China Chemistry, 2013, 56, 1263-1266.	8.2	4
75	Combining spin-adapted open-shell TD-DFT with spinâ€“orbit coupling. Molecular Physics, 2013, 111, 3741-3755.	1.7	85
76	Going beyond â€œno-pair relativistic quantum chemistryâ€• Journal of Chemical Physics, 2013, 139, 014108.	3.0	63
77	Body-fixed relativistic molecular Hamiltonian and its application to nuclear spin-rotation tensor. Journal of Chemical Physics, 2013, 138, 134104.	3.0	36
78	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
79	On the spin separation of algebraic two-component relativistic Hamiltonians. Journal of Chemical Physics, 2012, 137, 154114.	3.0	123
80	Relativistic explicit correlation: Coalescence conditions and practical suggestions. Journal of Chemical Physics, 2012, 136, 144117.	3.0	36
81	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.	3.0	31
82	A spin-adapted size-extensive state-specific multi-reference perturbation theory. I. Formal developments. Journal of Chemical Physics, 2012, 136, 024105.	3.0	43
83	Exact two-component relativistic theory for NMR parameters: General formulation and pilot application. Journal of Chemical Physics, 2012, 137, 174105.	3.0	54
84	Perspectives of relativistic quantum chemistry: the negative energy cat smiles. Physical Chemistry Chemical Physics, 2012, 14, 35-48.	2.8	72
85	Theoretical and numerical assessments of spin-flip time-dependent density functional theory. Journal of Chemical Physics, 2012, 136, 024107.	3.0	66
86	The 'big picture' of relativistic molecular quantum mechanics. AIP Conference Proceedings, 2012, , .	0.4	9
87	Special issue of Chemical Physics on recent advances and applications of relativistic quantum chemistry. Chemical Physics, 2012, 395, 1.	1.9	1
88	Fully relativistic theories and methods for NMR parameters. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	45
89	Fully relativistic theories and methods for NMR parameters. , 2012, , 187-203.		36
90	Linear-Scaling Time-Dependent Density Functional Theory Based on the Idea of â€œFrom Fragments to Moleculeâ€• Journal of Chemical Theory and Computation, 2011, 7, 3643-3660.	5.3	70

#	Article	IF	Citations
91	Spin-adapted open-shell time-dependent density functional theory. II. Theory and pilot application. Journal of Chemical Physics, 2011, 134, 134101.	3.0	68
92	Spin-adapted open-shell time-dependent density functional theory. III. An even better and simpler formulation. Journal of Chemical Physics, 2011, 135, 194106.	3.0	57
93	Comparison of restricted, unrestricted, inverse, and dual kinetic balances for four-component relativistic calculations. Theoretical Chemistry Accounts, 2011, 129, 423-436.	1.4	73
94	On the performance of the open-shell perturbation theory. Science China Chemistry, 2011, 54, 446-453.	8.2	7
95	Tuning mesomorphic properties and handedness of chiral calamitic liquid crystals by minimal modification of the effective core. Chirality, 2011, 23, E74-83.	2.6	4
96	Excited states of OsO₄: A comprehensive timeâ€dependent relativistic density functional theory study. Journal of Computational Chemistry, 2010, 31, 532-551.	3.3	19
97	SOLVATION ENERGY OF NONEQUILIBRIUM POLARIZATION: OLD QUESTION, NEW ANSWER. Journal of Theoretical and Computational Chemistry, 2010, 09, 23-37.	1.8	17
98	Ideas of relativistic quantum chemistry. Molecular Physics, 2010, 108, 1679-1706.	1.7	286
99	He@Mo6Cl8F6: A Stable Complex of Helium. Journal of Physical Chemistry A, 2010, 114, 646-651.	2.5	20
100	Spin-adapted open-shell random phase approximation and time-dependent density functional theory. I. Theory. Journal of Chemical Physics, 2010, 133, 064106.	3.0	68
101	Four-component relativistic theory for nuclear magnetic shielding: Magnetically balanced gauge-including atomic orbitals. Journal of Chemical Physics, 2009, 131, 244113.	3.0	79
102	Publisherâ€™s Note: â€œFour-component relativistic theory for NMR parameters: Unified formulation and numerical assessment of different approachesâ€•[J. Chem. Phys. 130, 144102 (2009)]. Journal of Chemical Physics, 2009, 131, 019902.	3.0	6
103	Comprehensive ab initio calculation and simulation on the lowâ€lying electronic states of TlX (X) Tj ETQq1 1 0.784314 rgBT /Ov	3.3	23
104	Time-dependent relativistic density functional study of Yb and YbO. Science in China Series B: Chemistry, 2009, 52, 1945-1953.	0.8	25
105	On the construction of Kramers paired double group symmetry functions. International Journal of Quantum Chemistry, 2009, 109, 2149-2167.	2.0	33
106	Excited states of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si14.gif" overflow="scroll"><mml:mrow><mml:msubsup><mml:mrow><mml:mtext>ReO</mml:mtext></mml:mrow><mml:mrow><mml:mn>4</mml:mn></mml:mrow> A comprehensive time-dependent relativistic density functional theory study. Chemical Physics, 2009, 356, 219-228.	1.9	26
107	Four-component relativistic theory for NMR parameters: Unified formulation and numerical assessment of different approaches. Journal of Chemical Physics, 2009, 130, 144102.	3.0	60
108	Exact two-component Hamiltonians revisited. Journal of Chemical Physics, 2009, 131, 031104.	3.0	298

#	Article	IF	Citations
109	Exact two-component relativistic theory for nuclear magnetic resonance parameters. Journal of Chemical Physics, 2009, 131, 081101.	3.0	56
110	Relativistic theory of nuclear magnetic resonance parameters in a Gaussian basis representation. Journal of Chemical Physics, 2009, 131, 044129.	3.0	37
111	Matrix formulation of direct perturbation theory of relativistic effects in a kinetically balanced basis. Chemical Physics, 2008, 349, 133-146.	1.9	5
112	Towards Nearâ€Infrared Chiroptically Switching Materials: Theoretical and Experimental Studies on Viologenâ€Containing 1,1â€²â€Binaphthyls. ChemPhysChem, 2008, 9, 1265-1269.	2.1	13
113	Making four- and two-component relativistic density functional methods fully equivalent based on the idea of â€œfrom atoms to moleculeâ€. Journal of Chemical Physics, 2007, 127, 104106.	3.0	210
114	Quasirelativistic theory. II. Theory at matrix level. Journal of Chemical Physics, 2007, 126, 114107.	3.0	149
115	Four-component relativistic theory for nuclear magnetic shielding constants: The orbital decomposition approach. Journal of Chemical Physics, 2007, 126, 081101.	3.0	64
116	Four-component relativistic theory for nuclear magnetic shielding constants: Critical assessments of different approaches. Journal of Chemical Physics, 2007, 126, 214101.	3.0	83
117	Theoretical study on the low-lying electronic states of NiH and NiAt. Journal of Computational Chemistry, 2007, 28, 2286-2298.	3.3	13
118	Ab initio investigation on electron transfer in molecular electronic devices: A minimal model study. Chemical Physics Letters, 2007, 439, 85-90.	2.6	3
119	Comprehensive theoretical studies on the low-lying electronic states of NiF, NiCl, NiBr, and NiI. Journal of Chemical Physics, 2006, 124, 154312.	3.0	30
120	NO2-catalyzed deep oxidation of methanol: Experimental and theoretical studies. Journal of Molecular Catalysis A, 2006, 252, 202-211.	4.8	20
121	Response to â€œComment on â€˜Quasirelativistic theory equivalent to fully relativistic theoryâ€™â€‰â€• [J. Chem. Phys. 123, 241102 (2005)]. Journal of Chemical Physics, 2006, 125, 107102.	3.0	23
122	Infinite-order quasirelativistic density functional method based on the exact matrix quasirelativistic theory. Journal of Chemical Physics, 2006, 125, 044102.	3.0	225
123	Quasirelativistic theory I. Theory in terms of a quasi-relativistic operator. Molecular Physics, 2006, 104, 2225-2240.	1.7	106
124	Quasirelativistic theory. , 2006, , 909-910.		1
125	A novel infinite-order quasirelativistic density functional theory. , 2006, , 919-922.		0
126	Benchmark four-component relativistic density functional calculations on Cu2, Ag2, and Au2. Chemical Physics, 2005, 311, 63-69.	1.9	22

#	Article	IF	Citations
127	Electronic coupling matrix elements of U-shaped donor-bridge-acceptor molecules and influence of mediated benzene solvent. Chemical Physics Letters, 2005, 414, 71-75.	2.6	3
128	Extensive theoretical studies on the low-lying electronic states of indium monochloride cation, InCl+. Journal of Computational Chemistry, 2005, 26, 106-113.	3.3	31
129	Time-dependent quasirelativistic density-functional theory based on the zeroth-order regular approximation. Journal of Chemical Physics, 2005, 123, 144101.	3.0	63
130	Time-dependent four-component relativistic density-functional theory for excitation energies. II. The exchange-correlation kernel. Journal of Chemical Physics, 2005, 123, 054102.	3.0	93
131	Quasirelativistic theory equivalent to fully relativistic theory. Journal of Chemical Physics, 2005, 123, 241102.	3.0	398
132	RELATIVISTIC DENSITY FUNCTIONAL THEORY: THE BDF PROGRAM PACKAGE. Recent Advances in Computational, 2004, , 257-282.	0.8	52
133	Time-dependent four-component relativistic density functional theory for excitation energies. Journal of Chemical Physics, 2004, 121, 6658-6666.	3.0	94
134	The Beijing Density Functional (BDF) Program Package: Methodologies and Applications. Journal of Theoretical and Computational Chemistry, 2003, 02, 257-272.	1.8	157
135	Comparison of Different Polarization Schemes in Openâ€shell Relativistic Density Functional Calculations. Journal of the Chinese Chemical Society, 2003, 50, 597-606.	1.4	70
136	On Relativity, Bonding, and Valence Electron Distribution. Journal of Physical Chemistry A, 2002, 106, 795-803.	2.5	10
137	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.	3.0	59
138	Molecular structure of diatomic lanthanide compounds. Science in China Series B: Chemistry, 2002, 45, 91.	0.8	37
139	Comprehensive relativisticab initio and density functional theory studies on PtH, PtF, PtCl, and Pt(NH3)2Cl2. Journal of Computational Chemistry, 2002, 23, 564-575.	3.3	28
140	Spectroscopic constants of Pb and Eka-lead compounds: comparison of different approaches. Advances in Quantum Chemistry, 2001, , 325-355.	0.8	65
141	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.	2.0	72
142	A small-core multiconfiguration Dirac-Hartree-Fock-adjusted pseudopotential for Tl - application to Tl X (X = F, Cl, Br, I). Theoretical Chemistry Accounts, 2000, 104, 22-28.	1.4	138
143	Comment on â€œFour-component relativistic density functional calculations of heavy diatomic moleculesâ€•[J. Chem. Phys. 112, 3499 (2000)]. Journal of Chemical Physics, 2000, 113, 2506-2507.	3.0	27
144	Relativistic MCSCF by means of quasidegenerate direct perturbation theory. I. Theory. Journal of Chemical Physics, 2000, 112, 3540-3558.	3.0	34

#	Article	IF	Citations
145	Relativistic MCSCF by means of quasidegenerate direct perturbation theory. II. Preliminary applications. Journal of Chemical Physics, 2000, 112, 3559-3571.	3.0	17
146	Relativistic ab initio and density functional theory calculations on the mercury fluorides: Is HgF4 thermodynamically stable?. Chemical Physics Letters, 1999, 302, 231-239.	2.6	40
147	Spectroscopic constants of gold and eka-gold (element 111) diatomic compounds: The importance of spinâ€“orbit coupling. Journal of Chemical Physics, 1999, 110, 3730-3735.	3.0	100
148	Calculated Properties of Lanthanocene Anions and the Unusual Electronic Structure of Their Neutral Counterparts. Inorganic Chemistry, 1998, 37, 1067-1072.	4.0	44
149	Orbital localization and delocalization effects in the U5f2configuration: Impurity problem. Physical Review B, 1998, 57, 10648-10654.	3.2	13
150	Benchmark calculations for lanthanide atoms: Calibration ofab initioand density-functional methods. Physical Review A, 1998, 57, 1721-1728.	2.5	55
151	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.	3.0	67
152	Ab initiopseudopotential and density-functional all-electron study of ionization and excitation energies of actinide atoms. Physical Review A, 1998, 58, 1103-1110.	2.5	74
153	Low-lying electronic states of lanthanocenes and actinocenes M(C8H8)2 (M=Nd, Tb, Yb, U). Journal of Chemical Physics, 1997, 107, 3584-3591.	3.0	66
154	A method for population and bonding analyses in calculations with extended basis sets. Theoretica Chimica Acta, 1997, 95, 81-95.	0.8	17
155	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.	1.4	247