Fan Wang

List of Publications by Year
in descending order

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115 papers	3,183 citations	186265 28 h-index	175258 52 g-index
118 all docs	118 docs citations	118 times ranked	2683 citing authors

#	Article	IF	Citations
1	Time-dependent density functional theory based on a noncollinear formulation of the exchange-correlation potential. Journal of Chemical Physics, 2004, 121, 12191.	3.0	243
2	The calculation of excitation energies based on the relativistic two-component zeroth-order regular approximation and time-dependent density-functional with full use of symmetry. Journal of Chemical Physics, 2005, 122, 204103.	3.0	238
3	A simplified relativistic time-dependent density-functional theory formalism for the calculations of excitation energies including spin-orbit coupling effect. Journal of Chemical Physics, 2005, 123, 154102.	3.0	209
4	Time-dependent density-functional theory for open systems. Physical Review B, 2007, 75, .	3.2	163
5	The Beijing Density Functional (BDF) Program Package: Methodologies and Applications. Journal of Theoretical and Computational Chemistry, 2003, 02, 257-272.	1.8	157
6	The performance of time-dependent density functional theory based on a noncollinear exchange-correlation potential in the calculations of excitation energies. Journal of Chemical Physics, 2005, 122, 074109.	3.0	121
7	LARMD: integration of bioinformatic resources to profile ligand-driven protein dynamics with a case on the activation of estrogen receptor. Briefings in Bioinformatics, 2020, 21, 2206-2218.	6.5	95
8	Flexible Conductive Polyimide Fiber/MXene Composite Film for Electromagnetic Interference Shielding and Joule Heating with Excellent Harsh Environment Tolerance. ACS Applied Materials & Interfaces, 2021, 13, 50368-50380.	8.0	85
9	BDF: A relativistic electronic structure program package. Journal of Chemical Physics, 2020, 152, 064113.	3.0	79
10	Closed-shell coupled-cluster theory with spin-orbit coupling. Journal of Chemical Physics, 2008, 129, 064113.	3.0	73
11	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
12	A novel role of the vacuolar calcium channel Yvc1 in stress response, morphogenesis and pathogenicity of Candida albicans. International Journal of Medical Microbiology, 2014, 304, 339-350.	3.6	63
13	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
14	RELATIVISTIC DENSITY FUNCTIONAL THEORY: THE BDF PROGRAM PACKAGE. Recent Advances in Computational, 2004, , 257-282.	0.8	52
15	ACID: a free tool for drug repurposing using consensus inverse docking strategy. Journal of Cheminformatics, 2019, 11, 73.	6.1	52
16	Theoretical study of the electronic spectra of square-planar platinum (II) complexes based on the two-component relativistic time-dependent density-functional theory. Journal of Chemical Physics, 2005, 123, 194102.	3.0	45
17	Equation-of-Motion Coupled-Cluster Theory for Excitation Energies of Closed-Shell Systems with Spinâ€“Orbit Coupling. Journal of Chemical Theory and Computation, 2014, 10, 5567-5576.	5.3	45
18	PADFrag: A Database Built for the Exploration of Bioactive Fragment Space for Drug Discovery. Journal of Chemical Information and Modeling, 2018, 58, 1725-1730.	5.4	45

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19	Equation-of-motion coupled-cluster method for ionized states with spin-orbit coupling. Journal of Chemical Physics, 2012, 136, 174102.	3.0	43
20	Use of noncollinear exchange-correlation potentials in multiplet resolutions by time-dependent density functional theory. International Journal of Quantum Chemistry, 2006, 106, 2545-2550.	2.0	40
21	Perturbative treatment of spin-orbit-coupling within spin-free exact two-component theory using equation-of-motion coupled-cluster methods. Journal of Chemical Physics, 2018, 148, 044108.	3.0	40
22	Symmetry exploitation in closed-shell coupled-cluster theory with spin-orbit coupling. Journal of Chemical Physics, 2011, 135, 034115.	3.0	39
23	Equation of motion coupled cluster method for electron attached states with spinâ€“orbit coupling. Chemical Physics Letters, 2012, 531, 236-241.	2.6	39
24	PlantSPEAD: a web resource towards comparatively analysing stressâ€responsive expression of splicingâ€related proteins in plant. Plant Biotechnology Journal, 2021, 19, 227-229.	8.3	38
25	Analytic energy gradients in closed-shell coupled-cluster theory with spin-orbit coupling. Journal of Chemical Physics, 2008, 129, 174110.	3.0	37
26	Theoretical Prediction of Rate Constants for Hydrogen Abstraction by OH, H, O, CH₃, and HO₂ Radicals from Toluene. Journal of Physical Chemistry A, 2016, 120, 3424-3432.	2.5	36
27	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
28	Skeletal mechanism generation for high-temperature oxidation of kerosene surrogates. Combustion and Flame, 2012, 159, 91-102.	5.2	32
29	Biochemical changes and defence responses during the development of peach gummosis caused by Lasiodiplodia theobromae. European Journal of Plant Pathology, 2014, 138, 195-207.	1.7	29
30	Sensitivity analysis based on intersection approach for mechanism reduction of cyclohexane. Combustion and Flame, 2016, 166, 55-65.	5.2	27
31	Analytic second derivatives in closed-shell coupled-cluster theory with spin-orbit coupling. Journal of Chemical Physics, 2009, 131, 164113.	3.0	26
32	Measuring the preference towards patient-centred communication with the Chinese-revised Patientâ€Practitioner Orientation Scale: a cross-sectional study among physicians and patients in clinical settings in Shanghai, China. BMJ Open, 2017, 7, e016902.	1.9	26
33	InsectiPAD: A Web Tool Dedicated to Exploring Physicochemical Properties and Evaluating Insecticide-Likeness of Small Molecules. Journal of Chemical Information and Modeling, 2019, 59, 630-635.	5.4	26
34	Synthesis of cellulose carbamates bearing regioselective substituents at 2,3- and 6-positions for efficient chromatographic enantioseparation. Journal of Chromatography A, 2018, 1572, 54-61.	3.7	24
35	Time-dependent density functional theory based Ehrenfest dynamics. Journal of Chemical Physics, 2011, 135, 044126.	3.0	23
36	Benchmark four-component relativistic density functional calculations on Cu2, Ag2, and Au2. Chemical Physics, 2005, 311, 63-69.	1.9	22

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37	Spinâ€“Orbit Effects in Closed-Shell Heavy and Superheavy Element Monohydrides and Monofluorides with Coupled-Cluster Theory. Journal of Physical Chemistry A, 2016, 120, 1231-1242.	2.5	22
38	Auto In Silico Ligand Directing Evolution to Facilitate the Rapid and Efficient Discovery of Drug Lead. IScience, 2020, 23, 101179.	4.1	22
39	Equation-of-motion coupled-cluster method for doubly ionized states with spin-orbit coupling. Journal of Chemical Physics, 2015, 142, 144109.	3.0	21
40	Identifying the Minimal Enzymes for Unusual Carbonâ€“Sulfur Bond Formation in Thienodolin Biosynthesis. ChemBioChem, 2016, 17, 799-803.	2.6	20
41	Delayed impact of natural climate solutions. Global Change Biology, 2021, 27, 215-217.	9.5	20
42	AIMMS suite: a web server dedicated for prediction of drug resistance on protein mutation. Briefings in Bioinformatics, 2018, , .	6.5	18
43	Chiral recognition ability of amylose derivatives bearing regioselectively different carbamate pendants at 2,3- and 6-positions. Carbohydrate Polymers, 2019, 218, 30-36.	10.2	18
44	Influence of the substituents on phenyl groups on enantioseparation property of amylose phenylcarbamates. Carbohydrate Polymers, 2020, 241, 116372.	10.2	18
45	Reduction of large-size combustion mechanisms of n-decane and n-dodecane with an improved sensitivity analysis method. Combustion and Flame, 2020, 222, 326-335.	5.2	17
46	<scp>HerbiPAD</scp>: a free web platform to comprehensively analyze constitutive property and herbicideâ€likeness to estimate chemical bioavailability. Pest Management Science, 2021, 77, 1273-1281.	3.4	17
47	Barrier heights of hydrogen-transfer reactions with diffusion quantum monte carlo method. Journal of Computational Chemistry, 2017, 38, 798-806.	3.3	16
48	Solvent effects for vertical absorption and emission processes in solution using a self-consistent state specific method based on constrained equilibrium thermodynamics. Physical Chemistry Chemical Physics, 2018, 20, 13178-13190.	2.8	16
49	Metagenomics analysis revealing the occurrence of antibiotic resistome in salt lakes. Science of the Total Environment, 2021, 790, 148262.	8.0	16
50	Theoretical investigation for spectroscopic constants of ground-state alkaline-earth dimers with high accuracy. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	15
51	Analytical energy gradient evaluation in relativistic and nonrelativistic density functional calculations. Journal of Computational Chemistry, 2002, 23, 920-927.	3.3	14
52	Flux Projection Tree Method for Mechanism Reduction. Energy & Fuels, 2014, 28, 5426-5433.	5.1	14
53	Coupled-cluster method for open-shell heavy-element systems with spin-orbit coupling. Journal of Chemical Physics, 2017, 146, 134108.	3.0	14
54	Why are male Chinese smokers unwilling to quit? A multicentre cross-sectional study on smoking rationalisation and intention to quit. BMJ Open, 2019, 9, e025285.	1.9	14

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55	An extensive study on skeletal mechanism reduction for the oxidation of C0â€“C4 fuels. Combustion and Flame, 2020, 214, 184-198.	5.2	13
56	Performance of the Diffusion Quantum Monte Carlo Method with a Single-Slater-Jastrow Trial Wavefunction Using Natural Orbitals and Density Functional Theory Orbitals on Atomization Energies of the Gaussian-2 Set. Journal of Physical Chemistry A, 2019, 123, 3809-3817.	2.5	12
57	Synthesis and Bioevaluation of Novel [¹⁸F]FDG-Conjugated 2-Nitroimidazole Derivatives for Tumor Hypoxia Imaging. Molecular Pharmaceutics, 2019, 16, 2118-2128.	4.6	12
58	Spinâ€“orbit coupling and electron correlation at various coupled-cluster levels for closed-shell diatomic molecules. Physical Chemistry Chemical Physics, 2013, 15, 17922.	2.8	11
59	Medical humanities play an important role in improving the doctor-patient relationship. BioScience Trends, 2017, 11, 134-137.	3.4	11
60	An Analytical Model of Seepage Field for Symmetrical Underwater Tunnels. Symmetry, 2018, 10, 273.	2.2	11
61	Theoretical Study on Reactions of Alkylperoxy Radicals. Journal of Physical Chemistry A, 2019, 123, 3949-3958.	2.5	11
62	Chinese Tobacco Industry Promotional Activity on the Microblog Weibo. PLoS ONE, 2014, 9, e99336.	2.5	11
63	Evaluation of Tunnel Face Stability Subjected to Seismic Load Based on the Non-associated Flow Rule. KSCE Journal of Civil Engineering, 2022, 26, 2478-2489.	1.9	11
64	A singularity excluded approximate expansion scheme in relativistic density functional theory. Theoretical Chemistry Accounts, 2002, 108, 53-60.	1.4	10
65	Template-Assisted Preparations of Crystalline Mo and Cu Nanonets. Journal of Physical Chemistry C, 2008, 112, 13121-13125.	3.1	10
66	Spin-orbit coupling with approximate equation-of-motion coupled-cluster method for ionization potential and electron attachment. Journal of Chemical Physics, 2016, 145, 154110.	3.0	10
67	PIIMS Server: A Web Server for Mutation Hotspot Scanning at the Proteinâ€“Protein Interface. Journal of Chemical Information and Modeling, 2021, 61, 14-20.	5.4	10
68	Numerical examination of performance of some exchange-correlation functionals for molecules containing heavy elements. Journal of Computational Chemistry, 2004, 25, 669-677.	3.3	9
69	Computational thermodynamic study on the complexes of Am(iii) with tridentate N-donor ligands. New Journal of Chemistry, 2015, 39, 7716-7729.	2.8	9
70	Fixed-Node Diffusion Quantum Monte Carlo Method on Dissociation Energies and Their Trends for Râ€“X Bonds (R = Me, Et, i-Pr, t-Bu). Journal of Physical Chemistry A, 2018, 122, 5050-5057.	2.5	9
71	A pre-targeting strategy for imaging glucose metabolism using technetium-99m labelled dibenzocyclooctyne derivative. Bioorganic and Medicinal Chemistry Letters, 2019, 29, 1791-1798.	2.2	9
72	Estimating nitrogen fates and gross transformations in bioretention systems with applications of 15N labeling methods. Chemosphere, 2021, 270, 129462.	8.2	9

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73	Excitation Energies of UO₂²⁺, NUO⁺, and NUN Based on Equation-of-Motion Coupled-Cluster Theory with Spinâ€“Orbit Coupling. Journal of Physical Chemistry A, 2017, 121, 3966-3975.	2.5	9
74	A new scheme for computer generation of molecular symmetry orbitals. Computational and Theoretical Chemistry, 2002, 586, 193-199.	1.5	8
75	Properties of closed-shell superheavy element hydrides and halides using coupled-cluster method and density functional theory with spin-orbit coupling. Journal of Chemical Physics, 2018, 148, 044304.	3.0	8
76	Single-precision open-shell CCSD and CCSD(T) calculations on graphics processing units. Physical Chemistry Chemical Physics, 2020, 22, 25103-25111.	2.8	8
77	Equation-of-motion coupled-cluster theory for double electron attachment with spinâ€“orbit coupling. Journal of Chemical Physics, 2020, 153, 214118.	3.0	8
78	Orbital-dependent magnetic properties of molecular cluster containing high-spin Co(II) ions. International Journal of Quantum Chemistry, 2009, 109, 3368-3378.	2.0	7
79	Study on Hydrogen Sensitivity of Zieglerâ€“Natta Catalysts with Novel Cycloalkoxy Silane Compounds as External Electron Donor. Polymers, 2016, 8, 433.	4.5	7
80	Middle-aged Driversâ€™ subjective categorization for combined alignments on mountainous freeways and their speed choices. Accident Analysis and Prevention, 2019, 127, 80-86.	5.7	7
81	Diffusion quantum Monte Carlo calculations with a recent generation of effective core potentials for ionization potentials and electron affinities. Physical Review A, 2019, 100, .	2.5	7
82	PTMdyna: exploring the influence of post-translation modifications on protein conformational dynamics. Briefings in Bioinformatics, 2022, 23, .	6.5	7
83	Acrylamide causes neurotoxicity by inhibiting glycolysis and causing the accumulation of carbonyl compounds in BV2 microglial cells. Food and Chemical Toxicology, 2022, 163, 112982.	3.6	7
84	â€˜Zhonghuaâ€™ tobacco advertisement in Shanghai: a descriptive study. Tobacco Control, 2014, 23, 389-394.	3.2	6
85	Skeletal Kinetic Model Generation for the Combustion of C₁-C₂ Fuels. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2016, 32, 1623-1633.	4.9	6
86	Investigation on terpolymer of ethylene/propylene/Ï‰-bromo-Î±-olefins catalyzed by titanium complexes. Journal of Materials Science, 2017, 52, 5981-5991.	3.7	6
87	Synthesis and bioevaluation of novel radioiodinated PEG-modified 2-nitroimidazole derivatives for tumor hypoxia imaging. Journal of Radioanalytical and Nuclear Chemistry, 2019, 321, 943-954.	1.5	6
88	Analytical energy gradients for ionized states using equation-of-motion coupled-cluster theory with spin-orbit coupling. Journal of Chemical Physics, 2019, 150, 154114.	3.0	6
89	Treating spin-orbit coupling at different levels in equation-of-motion coupled-cluster calculations. Molecular Physics, 2020, 118, e1785029.	1.7	6
90	G-quadruplexes in genomes of viruses infecting eukaryotes or prokaryotes are under different selection pressures from hosts. Journal of Genetics and Genomics, 2022, 49, 20-29.	3.9	6

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91	Reactive Molecular Dynamics Simulation on Thermal Decomposition of nâ€Heptane. Chinese Journal of Chemical Physics, 2013, 26, 211-219.	1.3	5
92	Analysis of a failure of the CC2 coupled-cluster method for bond lengths of SnO and PbO. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	5
93	Representations of electronic cigarettes in Chinese media. BMC Public Health, 2018, 18, 727.	2.9	5
94	Approximate equation-of-motion coupled-cluster methods for electron affinities of closed-shell molecules. Journal of Chemical Physics, 2020, 152, 124111.	3.0	5
95	Exploring the kinase-inhibitor fragment interaction space facilitates the discovery of kinase inhibitor overcoming resistance by mutations. Briefings in Bioinformatics, 2022, 23, .	6.5	5
96	Singletâ€“triplet gaps in diradicals obtained with diffusion quantum Monte Carlo using a Slaterâ€“Jastrow trial wavefunction with a minimum number of determinants. Physical Chemistry Chemical Physics, 2019, 21, 20422-20431.	2.8	4
97	Elevated KrÃ¼ppel-like factor 5 expression in spatiotemporal mouse lungs is similar to human congenital cystic adenomatoid malformation of the lungs. Journal of International Medical Research, 2018, 46, 2856-2865.	1.0	3
98	A corrected CIS(Dâˆž) method for valence and Rydberg excitation energies. Chemical Physics Letters, 2019, 730, 54-59.	2.6	3
99	Diffusion Monte Carlo method on small boron clusters using single- and multi- determinantâ€“Jastrow trial wavefunctions. Journal of Chemical Physics, 2021, 154, 024301.	3.0	3
100	Mode Coupling Analysis for a Mode Selective Coupler Using the Supermode Theory. Photonics, 2022, 9, 63.	2.0	3
101	Preparation of cellulose derivative bearing bulky 4â€(2â€benzothienyl)phenylcarbamate substituents as chiral stationary phase for enantioseparation. Chirality, 2022, 34, 701-710.	2.6	3
102	Magnetic Exchange Interaction in [BNITPhOPr] and [Cu(Cl₂CHCO₂)₂(NITpPy)₂(H₂O)]: A Density Functional Theory Study. Journal of the Chinese Chemical Society, 2003, 50, 645-653.	1.4	2
103	Equation-of-motion coupled-cluster method for ionised states with spin-orbit coupling using open-shell reference wavefunction. Molecular Physics, 2018, 116, 935-943.	1.7	2
104	Novel nonequilibrium solvation theory for calculating the vertical ionization energies of alkali metal cations and DNA bases in aqueous. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	2
105	Splittings of d8 configurations of late-transition metals with EOM-DIP-CCSD and FSCCSD methods. Journal of Chemical Physics, 2020, 152, 134105.	3.0	2
106	Energy correction and analytic energy gradients due to triples in CCSD(T) with spinâ€“orbit coupling on graphic processing units using single-precision data. Molecular Physics, 0, , .	1.7	2
107	Low-lying states of MX2 (M = Ag, Au; X = Cl, Br and I) with coupled-cluster approaches: effect of the basis set, high level correlation and spinâ€“orbit coupling. Physical Chemistry Chemical Physics, 2020, 22, 26178-26188.	2.8	2
108	Effects of ligands on excitation energies of [<scp>UO₂X₄</scp>]^{2â^’} and <scp>UO₂X₂</scp> (XÂ=ÂF, Cl) with the equationâ€ofâ€motion coupledâ€cluster theory. International Journal of Quantum Chemistry, 2022, 122, .	2.0	2

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109	Theoretical study on low-lying states of Ga2X (X = P, As) with coupled-cluster approaches. Physical Chemistry Chemical Physics, 2013, 15, 17929.	2.8	1
110	Stationary Points on Potential Energy Surface of Cyclic C3H3 with Coupled-Cluster Approaches and Density Functional Theory. Journal of Physical Chemistry A, 2021, 125, 4079-4088.	2.5	1
111	Theoretical Study on Reactions of Î±-Site Hydroxyethyl and Hydroxypropyl Radicals with O2. Journal of Physical Chemistry A, 2021, 125, 5423-5437.	2.5	1
112	Diffusion quantum Monte Carlo method on diradicals using single- and multi-determinant-Jastrow trial wavefunctions and different orbitals. Journal of Chemical Physics, 2022, 156, 124308.	3.0	1
113	Intermediate Hamiltonian Fock-space coupled-cluster theory for excitation energies, double ionization potentials, and double electron attachments with spinâ€“orbit coupling. Journal of Chemical Physics, 2022, 156, 114111.	3.0	1
114	An O(N) Time-Domain Method for Time-Dependent Density Functional Theory. , 2009, , .		0
115	Low-lying states of Tl2 and Nh2 with EOM-CC and FSCC methods. Chemical Physics Letters, 2021, 773, 138593.	2.6	0