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	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
2	PTMdyna: exploring the influence of post-translation modifications on protein conformational dynamics. Briefings in Bioinformatics, 2022, 23, .	6.5	7
3	Mode Coupling Analysis for a Mode Selective Coupler Using the Supermode Theory. Photonics, 2022, 9, 63.	2.0	3
4	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
5	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
6	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
7	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
8	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
9	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
10	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
11	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
12	<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
13	Delayed impact of natural climate solutions. Global Change Biology, 2021, 27, 215-217.	9.5	20
14	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
15	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
16	Estimating nitrogen fates and gross transformations in bioretention systems with applications of 15N labeling methods. Chemosphere, 2021, 270, 129462.	8.2	9
17	Low-lying states of Tl2 and Nh2 with EOM-CC and FSCC methods. Chemical Physics Letters, 2021, 773, 138593.	2.6	0
18	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

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19	Metagenomics analysis revealing the occurrence of antibiotic resistome in salt lakes. Science of the Total Environment, 2021, 790, 148262.	8.0	16
20	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
21	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
22	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
23	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
24	Single-precision open-shell CCSD and CCSD(T) calculations on graphics processing units. Physical Chemistry Chemical Physics, 2020, 22, 25103-25111.	2.8	8
25	Auto In Silico Ligand Directing Evolution to Facilitate the Rapid and Efficient Discovery of Drug Lead. IScience, 2020, 23, 101179.	4.1	22
26	Approximate equation-of-motion coupled-cluster methods for electron affinities of closed-shell molecules. Journal of Chemical Physics, 2020, 152, 124111.	3.0	5
27	Treating spin-orbit coupling at different levels in equation-of-motion coupled-cluster calculations. Molecular Physics, 2020, 118, e1785029.	1.7	6
28	Influence of the substituents on phenyl groups on enantioseparation property of amylose phenylcarbamates. Carbohydrate Polymers, 2020, 241, 116372.	10.2	18
29	BDF: A relativistic electronic structure program package. Journal of Chemical Physics, 2020, 152, 064113.	3.0	79
30	An extensive study on skeletal mechanism reduction for the oxidation of C0â€“C4 fuels. Combustion and Flame, 2020, 214, 184-198.	5.2	13
31	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
32	Equation-of-motion coupled-cluster theory for double electron attachment with spinâ€“orbit coupling. Journal of Chemical Physics, 2020, 153, 214118.	3.0	8
33	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
34	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
35	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
36	A corrected CIS(Dâˆž) method for valence and Rydberg excitation energies. Chemical Physics Letters, 2019, 730, 54-59.	2.6	3

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37	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
38	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
39	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
40	Theoretical Study on Reactions of Alkylperoxy Radicals. Journal of Physical Chemistry A, 2019, 123, 3949-3958.	2.5	11
41	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
42	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
43	Synthesis and Bioevaluation of Novel [¹⁸F]FDG-Conjugated 2-Nitroimidazole Derivatives for Tumor Hypoxia Imaging. Molecular Pharmaceutics, 2019, 16, 2118-2128.	4.6	12
44	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
45	ACID: a free tool for drug repurposing using consensus inverse docking strategy. Journal of Cheminformatics, 2019, 11, 73.	6.1	52
46	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
47	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
48	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
49	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
50	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
51	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
52	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
53	AIMMS suite: a web server dedicated for prediction of drug resistance on protein mutation. Briefings in Bioinformatics, 2018, , .	6.5	18
54	An Analytical Model of Seepage Field for Symmetrical Underwater Tunnels. Symmetry, 2018, 10, 273.	2.2	11

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55	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
56	Representations of electronic cigarettes in Chinese media. BMC Public Health, 2018, 18, 727.	2.9	5
57	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
58	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
59	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
60	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
61	Barrier heights of hydrogen-transfer reactions with diffusion quantum monte carlo method. Journal of Computational Chemistry, 2017, 38, 798-806.	3.3	16
62	Coupled-cluster method for open-shell heavy-element systems with spin-orbit coupling. Journal of Chemical Physics, 2017, 146, 134108.	3.0	14
63	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
64	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
65	Medical humanities play an important role in improving the doctor-patient relationship. BioScience Trends, 2017, 11, 134-137.	3.4	11
66	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
67	Study on Hydrogen Sensitivity of Zieglerâ€“Natta Catalysts with Novel Cycloalkoxy Silane Compounds as External Electron Donor. Polymers, 2016, 8, 433.	4.5	7
68	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
69	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
70	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
71	Identifying the Minimal Enzymes for Unusual Carbonâ€“Sulfur Bond Formation in Thienodolin Biosynthesis. ChemBioChem, 2016, 17, 799-803.	2.6	20
72	Sensitivity analysis based on intersection approach for mechanism reduction of cyclohexane. Combustion and Flame, 2016, 166, 55-65.	5.2	27

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73	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
74	Equation-of-motion coupled-cluster method for doubly ionized states with spin-orbit coupling. Journal of Chemical Physics, 2015, 142, 144109.	3.0	21
75	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
76	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
77	â€˜Zhonghuaâ€™ tobacco advertisement in Shanghai: a descriptive study. Tobacco Control, 2014, 23, 389-394.	3.2	6
78	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
79	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
80	Flux Projection Tree Method for Mechanism Reduction. Energy & Fuels, 2014, 28, 5426-5433.	5.1	14
81	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
82	Chinese Tobacco Industry Promotional Activity on the Microblog Weibo. PLoS ONE, 2014, 9, e99336.	2.5	11
83	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
84	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
85	Reactive Molecular Dynamics Simulation on Thermal Decomposition of nâ€Heptane. Chinese Journal of Chemical Physics, 2013, 26, 211-219.	1.3	5
86	Equation of motion coupled cluster method for electron attached states with spinâ€“orbit coupling. Chemical Physics Letters, 2012, 531, 236-241.	2.6	39
87	Equation-of-motion coupled-cluster method for ionized states with spin-orbit coupling. Journal of Chemical Physics, 2012, 136, 174102.	3.0	43
88	Skeletal mechanism generation for high-temperature oxidation of kerosene surrogates. Combustion and Flame, 2012, 159, 91-102.	5.2	32
89	Theoretical investigation for spectroscopic constants of ground-state alkaline-earth dimers with high accuracy. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	15
90	Time-dependent density functional theory based Ehrenfest dynamics. Journal of Chemical Physics, 2011, 135, 044126.	3.0	23

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91	Symmetry exploitation in closed-shell coupled-cluster theory with spin-orbit coupling. Journal of Chemical Physics, 2011, 135, 034115.	3.0	39
92	An O(N) Time-Domain Method for Time-Dependent Density Functional Theory. , 2009, , .		0
93	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
94	Analytic second derivatives in closed-shell coupled-cluster theory with spin-orbit coupling. Journal of Chemical Physics, 2009, 131, 164113.	3.0	26
95	Closed-shell coupled-cluster theory with spin-orbit coupling. Journal of Chemical Physics, 2008, 129, 064113.	3.0	73
96	Template-Assisted Preparations of Crystalline Mo and Cu Nanonets. Journal of Physical Chemistry C, 2008, 112, 13121-13125.	3.1	10
97	Analytic energy gradients in closed-shell coupled-cluster theory with spin-orbit coupling. Journal of Chemical Physics, 2008, 129, 174110.	3.0	37
98	Time-dependent density-functional theory for open systems. Physical Review B, 2007, 75, .	3.2	163
99	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
100	Benchmark four-component relativistic density functional calculations on Cu2, Ag2, and Au2. Chemical Physics, 2005, 311, 63-69.	1.9	22
101	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
102	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
103	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
104	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
105	RELATIVISTIC DENSITY FUNCTIONAL THEORY: THE BDF PROGRAM PACKAGE. Recent Advances in Computational, 2004, , 257-282.	0.8	52
106	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
107	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
108	The Beijing Density Functional (BDF) Program Package: Methodologies and Applications. Journal of Theoretical and Computational Chemistry, 2003, 02, 257-272.	1.8	157

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109	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
110	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
111	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
112	Analytical energy gradient evaluation in relativistic and nonrelativistic density functional calculations. Journal of Computational Chemistry, 2002, 23, 920-927.	3.3	14
113	A singularity excluded approximate expansion scheme in relativistic density functional theory. Theoretical Chemistry Accounts, 2002, 108, 53-60.	1.4	10
114	A new scheme for computer generation of molecular symmetry orbitals. Computational and Theoretical Chemistry, 2002, 586, 193-199.	1.5	8
115	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