Jin-Feng Liu

List of Publications by Year
in descending order

39	1,255	361413 20	361022 35
papers	citations	h-index	g-index

40	40	40	1061
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The mitochondrial Î²-oxidation enzyme HADHA restrains hepatic glucagon response by promoting Î²-hydroxybutyrate production. Nature Communications, 2022, 13, 386.	12.8	13
2	Ionization of D571 Is Coupled with SARS-CoV-2 Spike Up/Down Equilibrium Revealing the pH-Dependent Allosteric Mechanism of Receptor-Binding Domains. Journal of Physical Chemistry B, 2022, 126, 4828-4839.	2.6	3
3	Toward High-level Machine Learning Potential for Water Based on Quantum Fragmentation and Neural Networks. Journal of Physical Chemistry A, 2022, 126, 3926-3936.	2.5	11
4	Ab initio determination of crystal stability of di-p-tolyl disulfide. Scientific Reports, 2021, 11, 7076.	3.3	4
5	Directional Proton Transfer in the Reaction of the Simplest Criegee Intermediate with Water Involving the Formation of Transient H₃O⁺. Journal of Physical Chemistry Letters, 2021, 12, 3379-3386.	4.6	16
6	Lanthanide Metalâ€“Organic Framework-Based Fluorescent Sensor Arrays to Discriminate and Quantify Ingredients of Natural Medicine. Langmuir, 2021, 37, 5321-5328.	3.5	15
7	Effect of Pterostilbene, a Natural Derivative of Resveratrol, in the Treatment of Colorectal Cancer through Top1/Tdp1-Mediated DNA Repair Pathway. Cancers, 2021, 13, 4002.	3.7	19
8	Towards complete assignment of the infrared spectrum of the protonated water cluster H+(H2O)21. Nature Communications, 2021, 12, 6141.	12.8	35
9	Ab initio molecular dynamics simulation of liquid water with fragment-based quantum mechanical approach under periodic boundary conditions. Chinese Journal of Chemical Physics, 2021, 34, 761-768.	1.3	1
10	Quantitative Prediction of Aggregationâ€Induced Emission: A Full Quantum Mechanical Approach to the Optical Spectra. Angewandte Chemie, 2020, 132, 11647-11652.	2.0	3
11	Fragment-based quantum mechanical approach to biomolecules, molecular clusters, molecular crystals and liquids. Physical Chemistry Chemical Physics, 2020, 22, 12341-12367.	2.8	38
12	Quantitative Prediction of Aggregationâ€Induced Emission: A Full Quantum Mechanical Approach to the Optical Spectra. Angewandte Chemie - International Edition, 2020, 59, 11550-11555.	13.8	23
13	Phase Transition of Ice at High Pressures and Low Temperatures. Molecules, 2020, 25, 486.	3.8	3
14	QM Implementation in Drug Design: Does It Really Help?. Methods in Molecular Biology, 2020, 2114, 19-35.	0.9	2
15	Improving proteinâ€“ligand binding prediction by considering the bridging water molecules in Autodock. Journal of Theoretical and Computational Chemistry, 2019, 18, 1950027.	1.8	2
16	Crystal Structure Optimization and Gibbs Free Energy Comparison of Five Sulfathiazole Polymorphs by the Embedded Fragment QM Method at the DFT Level. Crystals, 2019, 9, 256.	2.2	7
17	Prediction of Excited-State Properties of Oligoacene Crystals Using Fragment-Based Quantum Mechanical Method. Journal of Physical Chemistry A, 2019, 123, 5407-5417.	2.5	18
18	Stability, Vibrations, and Diffusion of Hydrogen Gas in Clathrate Hydrates: Insights from Ab Initio Calculations on Condensed-Phase Crystalline Structures. Journal of Physical Chemistry C, 2019, 123, 12052-12061.	3.1	20

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19	Predicting the phase diagram of solid carbon dioxide at high pressure from first principles. Npj Quantum Materials, 2019, 4, .	5.2	29
20	G1 phase cell cycle arrest in NSCLC in response to LZ-106, an analog of enoxacin, is orchestrated through ROS overproduction in a P53-dependent manner. Carcinogenesis, 2019, 40, 131-144.	2.8	9
21	A Coupled Ionization-Conformational Equilibrium Is Required To Understand the Properties of Ionizable Residues in the Hydrophobic Interior of Staphylococcal Nuclease. Journal of the American Chemical Society, 2018, 140, 1639-1648.	13.7	22
22	Fragmentâ€based quantum mechanical calculation of proteinâ€“protein binding affinities. Journal of Computational Chemistry, 2018, 39, 1617-1628.	3.3	23
23	Hydrogen-bond structure dynamics in bulk water: insights from ab initio simulations with coupled cluster theory. Chemical Science, 2018, 9, 2065-2073.	7.4	98
24	Probing the Ion-Specific Effects at the Water/Air Interface and Water-Mediated Ion Pairing in Sodium Halide Solution with Ab Initio Molecular Dynamics. Journal of Physical Chemistry B, 2018, 122, 10202-10209.	2.6	19
25	Structure of liquid water â€“ a dynamical mixture of tetrahedral and â€˜ring-and-chainâ€™ like structures. Physical Chemistry Chemical Physics, 2017, 19, 11931-11936.	2.8	50
26	Fragment Quantum Mechanical Method for Large-Sized Ionâ€“Water Clusters. Journal of Chemical Theory and Computation, 2017, 13, 2021-2034.	5.3	54
27	Vibrational Signatures of Isomeric Lithiated N-acetyl-D-hexosamines by Gas-Phase Infrared Multiple-Photon Dissociation (IRMPD) Spectroscopy. Journal of the American Society for Mass Spectrometry, 2017, 28, 539-550.	2.8	26
28	Differential regulation of baicalin and scutellarin on AMPK and Akt in promoting adipose cell glucose disposal. Biochimica Et Biophysica Acta - Molecular Basis of Disease, 2017, 1863, 598-606.	3.8	27
29	Accurate prediction of energetic properties of ionic liquid clusters using a fragment-based quantum mechanical method. Physical Chemistry Chemical Physics, 2017, 19, 20657-20666.	2.8	35
30	Ginsenoside Rg1 Inhibits Glucagon-Induced Hepatic Gluconeogenesis through Akt-FoxO1 Interaction. Theranostics, 2017, 7, 4001-4012.	10.0	104
31	PBSA_E: A PBSA-Based Free Energy Estimator for Proteinâ€“Ligand Binding Affinity. Journal of Chemical Information and Modeling, 2016, 56, 854-861.	5.4	12
32	Fragment quantum chemical approach to geometry optimization and vibrational spectrum calculation of proteins. Physical Chemistry Chemical Physics, 2016, 18, 1864-1875.	2.8	60
33	Calculation of proteinâ€“ligand binding affinities based on a fragment quantum mechanical method. RSC Advances, 2015, 5, 107020-107030.	3.6	47
34	Quantum Fragment Based ab Initio Molecular Dynamics for Proteins. Journal of Chemical Theory and Computation, 2015, 11, 5897-5905.	5.3	59
35	Novel theoretically designed HIV-1 non-nucleoside reverse transcriptase inhibitors derived from nevirapine. Journal of Molecular Modeling, 2014, 20, 2451.	1.8	3
36	Fragment Quantum Mechanical Calculation of Proteins and Its Applications. Accounts of Chemical Research, 2014, 47, 2748-2757.	15.6	173

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37	Improving the Scoring of Proteinâ€“Ligand Binding Affinity by Including the Effects of Structural Water and Electronic Polarization. Journal of Chemical Information and Modeling, 2013, 53, 1306-1314.	5.4	39
38	Electrostatically Embedded Generalized Molecular Fractionation with Conjugate Caps Method for Full Quantum Mechanical Calculation of Protein Energy. Journal of Physical Chemistry A, 2013, 117, 7149-7161.	2.5	93
39	An improved fragment-based quantum mechanical method for calculation of electrostatic solvation energy of proteins. Journal of Chemical Physics, 2013, 139, 214104.	3.0	34