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	Fragment Quantum Mechanical Calculation of Proteins and Its Applications. Accounts of Chemical Research, 2014, 47, 2748-2757.	15.6	173
2	Ginsenoside Rg1 Inhibits Glucagon-Induced Hepatic Gluconeogenesis through Akt-FoxO1 Interaction. Theranostics, 2017, 7, 4001-4012.	10.0	104
3	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
4	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
5	Fragment quantum chemical approach to geometry optimization and vibrational spectrum calculation of proteins. Physical Chemistry Chemical Physics, 2016, 18, 1864-1875.	2.8	60
6	Quantum Fragment Based ab Initio Molecular Dynamics for Proteins. Journal of Chemical Theory and Computation, 2015, 11, 5897-5905.	5.3	59
7	Fragment Quantum Mechanical Method for Large-Sized Ionâ€“Water Clusters. Journal of Chemical Theory and Computation, 2017, 13, 2021-2034.	5.3	54
8	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
9	Calculation of proteinâ€“ligand binding affinities based on a fragment quantum mechanical method. RSC Advances, 2015, 5, 107020-107030.	3.6	47
10	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
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	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
13	Towards complete assignment of the infrared spectrum of the protonated water cluster H+(H2O)21. Nature Communications, 2021, 12, 6141.	12.8	35
14	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
15	Predicting the phase diagram of solid carbon dioxide at high pressure from first principles. Npj Quantum Materials, 2019, 4, .	5.2	29
16	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
17	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
18	Fragmentâ€based quantum mechanical calculation of proteinâ€“protein binding affinities. Journal of Computational Chemistry, 2018, 39, 1617-1628.	3.3	23

#	Article	IF	Citations
19	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
20	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
21	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
22	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
23	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
24	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
25	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
26	Lanthanide Metalâ€“Organic Framework-Based Fluorescent Sensor Arrays to Discriminate and Quantify Ingredients of Natural Medicine. Langmuir, 2021, 37, 5321-5328.	3.5	15
27	The mitochondrial Î²-oxidation enzyme HADHA restrains hepatic glucagon response by promoting Î²-hydroxybutyrate production. Nature Communications, 2022, 13, 386.	12.8	13
28	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
29	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
30	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
31	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
32	Ab initio determination of crystal stability of di-p-tolyl disulfide. Scientific Reports, 2021, 11, 7076.	3.3	4
33	Novel theoretically designed HIV-1 non-nucleoside reverse transcriptase inhibitors derived from nevirapine. Journal of Molecular Modeling, 2014, 20, 2451.	1.8	3
34	Quantitative Prediction of Aggregationâ€Induced Emission: A Full Quantum Mechanical Approach to the Optical Spectra. Angewandte Chemie, 2020, 132, 11647-11652.	2.0	3
35	Phase Transition of Ice at High Pressures and Low Temperatures. Molecules, 2020, 25, 486.	3.8	3
36	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

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37	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
38	QM Implementation in Drug Design: Does It Really Help?. Methods in Molecular Biology, 2020, 2114, 19-35.	0.9	2
39	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