Xiao He

List of Publications by Citations

120 papers	3,506 citations	32 h-index	56 g-index
134 ext. papers	4,393 ext. citations	5.9 avg, IF	5.97 L-index

#	Paper	IF	Citations
120	MN15: A Kohn-Sham global-hybrid exchange-correlation density functional with broad accuracy for multi-reference and single-reference systems and noncovalent interactions. *Chemical Science*, **2016**, 7, 5032-5051	9.4	491
119	MN15-L: A New Local Exchange-Correlation Functional for Kohn-Sham Density Functional Theory with Broad Accuracy for Atoms, Molecules, and Solids. *Journal of Chemical Theory and Computation*, **2016**, 12, 1280-93	6.4	246
118	Fragment quantum mechanical calculation of proteins and its applications. *Accounts of Chemical Research*, **2014**, 47, 2748-57	24.3	129
117	Revised M06-L functional for improved accuracy on chemical reaction barrier heights, noncovalent interactions, and solid-state physics. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 8487-8492	11.5	120
116	Divide-and-Conquer Hartree-Fock Calculations on Proteins. *Journal of Chemical Theory and Computation*, **2010**, 6, 405-411	6.4	117
115	Formal Estimation of Errors in Computed Absolute Interaction Energies of Protein-ligand Complexes. *Journal of Chemical Theory and Computation*, **2011**, 7, 790-797	6.4	116
114	A new method for direct calculation of total energy of protein. *Journal of Chemical Physics*, **2005**, 122, 31103	3.9	103
113	Nonseparable exchange-correlation functional for molecules, including homogeneous catalysis involving transition metals. *Physical Chemistry Chemical Physics*, **2015**, 17, 12146-60	3.6	92
112	Protein NMR chemical shift calculations based on the automated fragmentation QM/MM approach. *Journal of Physical Chemistry B*, **2009**, 113, 10380-8	3.4	79
111	The generalized molecular fractionation with conjugate caps/molecular mechanics method for direct calculation of protein energy. *Journal of Chemical Physics*, **2006**, 124, 184703	3.9	77
110	Electrostatically embedded generalized molecular fractionation with conjugate caps method for full quantum mechanical calculation of protein energy. *Journal of Physical Chemistry A*, **2013**, 117, 7149-61	2.8	75
109	Further analysis and comparative study of intermolecular interactions using dimers from the S22 database. *Journal of Chemical Physics*, **2009**, 131, 065102	3.9	75
108	Hydrogen-bond structure dynamics in bulk water: insights from simulations with coupled cluster theory. *Chemical Science*, **2018**, 9, 2065-2073	9.4	68
107	Revised M06 density functional for main-group and transition-metal chemistry. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 10257-10262	11.5	67
106	Fragment density functional theory calculation of NMR chemical shifts for proteins with implicit solvation. *Physical Chemistry Chemical Physics*, **2012**, 14, 7837-45	3.6	66
105	Ab initio molecular crystal structures, spectra, and phase diagrams. *Accounts of Chemical Research*, **2014**, 47, 2721-30	24.3	65
104	Second-order many-body perturbation study of ice Ih. *Journal of Chemical Physics*, **2012**, 137, 204505	3.9	65

103	Automated Fragmentation QM/MM Calculation of Amide Proton Chemical Shifts in Proteins with Explicit Solvent Model. *Journal of Chemical Theory and Computation*, **2013**, 9, 2104-14	6.4	63
102	Importance of dispersion and electron correlation in ab initio protein folding. *Journal of Physical Chemistry B*, **2009**, 113, 5290-300	3.4	61
101	Quantum computational analysis for drug resistance of HIV-1 reverse transcriptase to nevirapine through point mutations. *Proteins: Structure, Function and Bioinformatics*, **2005**, 61, 423-32	4.2	49
100	Effect of strong electric field on the conformational integrity of insulin. *Journal of Physical Chemistry A*, **2014**, 118, 8942-52	2.8	47
99	Revised M11 Exchange-Correlation Functional for Electronic Excitation Energies and Ground-State Properties. *Journal of Physical Chemistry A*, **2019**, 123, 2966-2990	2.8	45
98	Fragment quantum chemical approach to geometry optimization and vibrational spectrum calculation of proteins. *Physical Chemistry Chemical Physics*, **2016**, 18, 1864-75	3.6	45
97	Quantum Fragment Based ab Initio Molecular Dynamics for Proteins. *Journal of Chemical Theory and Computation*, **2015**, 11, 5897-905	6.4	43
96	Quantum study of mutational effect in binding of efavirenz to HIV-1 RT. *Proteins: Structure, Function and Bioinformatics*, **2005**, 59, 489-95	4.2	42
95	The energy computation paradox and ab initio protein folding. *PLoS ONE*, **2011**, 6, e18868	3.7	41
94	Fragment Quantum Mechanical Method for Large-Sized Ion-Water Clusters. *Journal of Chemical Theory and Computation*, **2017**, 13, 2021-2034	6.4	39
93	Structure of liquid water - a dynamical mixture of tetrahedral and “ring-and-chain”like structures. *Physical Chemistry Chemical Physics*, **2017**, 19, 11931-11936	3.6	37
92	AFNMR: automated fragmentation quantum mechanical calculation of NMR chemical shifts for biomolecules. *Journal of Biomolecular NMR*, **2015**, 63, 125-39	3	36
91	Improving the scoring of protein-ligand binding affinity by including the effects of structural water and electronic polarization. *Journal of Chemical Information and Modeling*, **2013**, 53, 1306-14	6.1	34
90	AIE-Active Chiral [3]Rotaxanes with Switchable Circularly Polarized Luminescence. *Angewandte Chemie - International Edition*, **2021**, 60, 9507-9515	16.4	33
89	Calculation of protein–ligand binding affinities based on a fragment quantum mechanical method. *RSC Advances*, **2015**, 5, 107020-107030	3.7	32
88	Acteoside Binds to Caspase-3 and Exerts Neuroprotection in the Rotenone Rat Model of Parkinson’s Disease. *PLoS ONE*, **2016**, 11, e0162696	3.7	30
87	Accurate prediction of energetic properties of ionic liquid clusters using a fragment-based quantum mechanical method. *Physical Chemistry Chemical Physics*, **2017**, 19, 20657-20666	3.6	28
86	Conformational variability of benzamidinium-based inhibitors. *Journal of the American Chemical Society*, **2009**, 131, 7742-54	16.4	28

85	An improved fragment-based quantum mechanical method for calculation of electrostatic solvation energy of proteins. *Journal of Chemical Physics*, **2013**, 139, 214104	3.9	27
84	On the Kohn-Luttinger conundrum. *Journal of Chemical Physics*, **2013**, 138, 204112	3.9	23
83	Anisotropic Gas Separation in Oriented ZIF-95 Membranes Prepared by Vapor-Assisted In-Plane Epitaxial Growth. *Angewandte Chemie - International Edition*, **2020**, 59, 20858-20862	16.4	23
82	Predicting the phase diagram of solid carbon dioxide at high pressure from first principles. *Npj Quantum Materials*, **2019**, 4,	5	21
81	Second-order many-body perturbation theory: an eternal frontier. *Journal of Physical Chemistry A*, **2014**, 118, 655-72	2.8	21
80	Multiconfiguration Pair-Density Functional Theory Is Free From Delocalization Error. *Journal of Physical Chemistry Letters*, **2017**, 8, 5616-5620	6.4	21
79	Predicting mutation-induced Stark shifts in the active site of a protein with a polarized force field. *Journal of Physical Chemistry A*, **2013**, 117, 6015-23	2.8	21
78	How Well Can the M06 Suite of Functionals Describe the Electron Densities of Ne, Ne, and Ne?. *Journal of Chemical Theory and Computation*, **2017**, 13, 6068-6077	6.4	19
77	Finite-temperature second-order many-body perturbation and Hartree-Fock theories for one-dimensional solids: an application to Peierls and charge-density-wave transitions in conjugated polymers. *Journal of Chemical Physics*, **2014**, 140, 024702	3.9	17
76	Accurate benchmark calculations on the gas-phase basicities of small molecules. *Journal of Physical Chemistry A*, **2009**, 113, 10096-103	2.8	17
75	Full QM Calculation of RNA Energy Using Electrostatically Embedded Generalized Molecular Fractionation with Conjugate Caps Method. *Journal of Physical Chemistry A*, **2017**, 121, 2503-2514	2.8	16
74	Fragment-based quantum mechanical approach to biomolecules, molecular clusters, molecular crystals and liquids. *Physical Chemistry Chemical Physics*, **2020**, 22, 12341-12367	3.6	16
73	M06-SX screened-exchange density functional for chemistry and solid-state physics. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 2294-2301	11.5	16
72	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	16.4	16
71	Prediction of Excited-State Properties of Oligoacene Crystals Using Fragment-Based Quantum Mechanical Method. *Journal of Physical Chemistry A*, **2019**, 123, 5407-5417	2.8	15
70	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	3.8	15
69	Combining the Fragmentation Approach and Neural Network Potential Energy Surfaces of Fragments for Accurate Calculation of Protein Energy. *Journal of Physical Chemistry B*, **2020**, 124, 3027-3035	3.4	15
68	Quantitative Prediction of Aggregation-Induced Emission: A Full Quantum Mechanical Approach to the Optical Spectra. *Angewandte Chemie - International Edition*, **2020**, 59, 11550-11555	16.4	14

67	Fragment-based quantum mechanical calculation of protein-protein binding affinities. *Journal of Computational Chemistry*, **2018**, 39, 1617-1628	3.5	14
66	Rational Crystal Polymorph Design of Olanzapine. *Crystal Growth and Design*, **2019**, 19, 2388-2395	3.5	13
65	Computational search for aflatoxin binding proteins. *Chemical Physics Letters*, **2017**, 685, 1-8	2.5	13
64	Polymer-supported graphene□TiO2 doped with nonmetallic elements with enhanced photocatalytic reaction under visible light. *Journal of Materials Science*, **2020**, 55, 1577-1591	4.3	13
63	From CuFeS to BaCuFeGeS: rational band gap engineering achieves large second-harmonic-generation together with high laser damage threshold. *Chemical Communications*, **2019**, 55, 14510-14513	5.8	13
62	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	3.4	13
61	Fragment Quantum Mechanical Method for Excited States of Proteins: Development and Application to the Green Fluorescent Protein. *Journal of Chemical Theory and Computation*, **2020**, 16, 5174-5188	6.4	12
60	Quantum Mechanical Study of Vicinal J Spin-Spin Coupling Constants for the Protein Backbone. *Journal of Chemical Theory and Computation*, **2013**, 9, 4653-9	6.4	12
59	M11plus: A Range-Separated Hybrid Meta Functional with Both Local and Rung-3.5 Correlation Terms and High Across-the-Board Accuracy for Chemical Applications. *Journal of Chemical Theory and Computation*, **2019**, 15, 4804-4815	6.4	11
58	Quantum mechanical calculation of electric fields and vibrational Stark shifts at active site of human aldose reductase. *Journal of Chemical Physics*, **2015**, 143, 184111	3.9	10
57	AIE-Active Chiral [3]Rotaxanes with Switchable Circularly Polarized Luminescence. *Angewandte Chemie*, **2021**, 133, 9593-9601	3.6	10
56	DeepBSP-a Machine Learning Method for Accurate Prediction of Protein-Ligand Docking Structures. *Journal of Chemical Information and Modeling*, **2021**, 61, 2231-2240	6.1	10
55	A systematic study on RNA NMR chemical shift calculation based on the automated fragmentation QM/MM approach. *RSC Advances*, **2016**, 6, 108590-108602	3.7	10
54	A Fragment Quantum Mechanical Method for Metalloproteins. *Journal of Chemical Theory and Computation*, **2019**, 15, 1430-1439	6.4	9
53	A coupled two-dimensional main chain torsional potential for protein dynamics: generation and implementation. *Journal of Molecular Modeling*, **2013**, 19, 3647-57	2	9
52	Comparison of quantum and mixed quantum□classical semirigid vibrating rotor target studies for isotopic reactions H(D,T)+CH4-HH(D,T)+CH3. *Journal of Chemical Physics*, **2003**, 119, 9455-9460	3.9	9
51	Anisotropic Gas Separation in Oriented ZIF-95 Membranes Prepared by Vapor-Assisted In-Plane Epitaxial Growth. *Angewandte Chemie*, **2020**, 132, 21044-21048	3.6	9
50	PBSA_E: A PBSA-Based Free Energy Estimator for Protein-Ligand Binding Affinity. *Journal of Chemical Information and Modeling*, **2016**, 56, 854-61	6.1	9

49	Exploring Protein Structures by DNP-Enhanced Methyl Solid-State NMR Spectroscopy. *Journal of the American Chemical Society*, **2019**, 141, 19888-19901	16.4	9
48	Automated Fragmentation QM/MM Calculation of NMR Chemical Shifts for Protein-Ligand Complexes. *Frontiers in Chemistry*, **2018**, 6, 150	5	7
47	Benchmark study of ionization potentials and electron affinities of armchair single-walled carbon nanotubes using density functional theory. *Journal of Physics Condensed Matter*, **2018**, 30, 215501	1.8	7
46	An Ab Initio QM/MM Study of the Electrostatic Contribution to Catalysis in the Active Site of Ketosteroid Isomerase. *Molecules*, **2018**, 23,	4.8	7
45	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	2.3	6
44	Structure, mechanism, and enantioselectivity shifting of lipase LipK107 with a simple way. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2014**, 1844, 1183-92	4	6
43	Towards complete assignment of the infrared spectrum of the protonated water cluster H(HO). *Nature Communications*, **2021**, 12, 6141	17.4	6
42	Ab initio-enabled phase transition prediction of solid carbon dioxide at ultra-high temperatures.. *RSC Advances*, **2019**, 10, 236-243	3.7	6
41	Atmospheric Kinetics: Bimolecular Reactions of Carbonyl Oxide by a Triple-Level Strategy. *Journal of the American Chemical Society*, **2021**, 143, 8402-8413	16.4	6
40	Assessing the performance of popular QM methods for calculation of conformational energies of trialanine. *Chemical Physics Letters*, **2016**, 652, 136-141	2.5	6
39	Functional roles of tyrosine 185 during the bacteriorhodopsin photocycle as revealed by in situ spectroscopic studies. *Biochimica Et Biophysica Acta - Bioenergetics*, **2018**, 1859, 1006-1014	4.6	6
38	Syntheses, structures, optical properties, and electronic structures of Ba6Cu2GSn4S16 (G = Fe, Ni) and Sr6D2FeSn4S16 (D = Cu, Ag). *Journal of Solid State Chemistry*, **2019**, 272, 69-77	3.3	5
37	Correction of erroneously packed proteinβ side chains in the NMR structure based on ab initio chemical shift calculations. *Physical Chemistry Chemical Physics*, **2014**, 16, 18163-9	3.6	5
36	Ab initio Quantum Mechanics/Molecular Mechanics Molecular Dynamics Simulation of CO in the Heme Distal Pocket of Myoglobin *Chinese Journal of Chemical Physics*, **2017**, 30, 705-716	0.9	5
35	Room-temperature dynamic nuclear polarization enhanced NMR spectroscopy of small biological molecules in water. *Nature Communications*, **2021**, 12, 6880	17.4	5
34	Ultrasensitive Sensing of Volatile Organic Compounds Using a Cu-Doped SnO -NiO p-n Heterostructure That Shows Significant Raman Enhancement*. *Angewandte Chemie - International Edition*, **2021**, 60, 26260-26267	16.4	5
33	Elimination of Grain Boundary Defects in Zeolitic Imidazolate Framework ZIF-95 Membrane via Solvent-Free Secondary Growth. *Angewandte Chemie - International Edition*, **2021**, 60, 25463-25467	16.4	5
32	A Semiautomated Structure-Based Method To Predict Substrates of Enzymes via Molecular Docking: A Case Study with Candida antarctica Lipase B. *Journal of Chemical Information and Modeling*, **2016**, 56, 1979-1994	6.1	4

31	Low-Temperature Polymorphic Transformation of ꞵLactam Antibiotics. *Crystals*, **2019**, 9, 460	2.3	3
30	Quantitative Prediction of Aggregation-Induced Emission: A Full Quantum Mechanical Approach to the Optical Spectra. *Angewandte Chemie*, **2020**, 132, 11647-11652	3.6	3
29	Ab Initio Prediction of the Phase Transition for Solid Ammonia at High Pressures. *Scientific Reports*, **2020**, 10, 7546	4.9	3
28	Binding mode of chitin and TLR2 via molecular docking and dynamics simulation. *Molecular Simulation*, **2016**, 42, 936-941	2	3
27	Reaction mechanisms of CO oxidation on cationic, neutral, and anionic X-O-Cu (X = Au, Ag) clusters. *Chemical Physics Letters*, **2017**, 686, 116-123	2.5	3
26	MFCC-Based Fragmentation Methods for Biomolecules **2017**, 323-348		3
25	Ab initio Ice, Dry Ice, and Liquid Water **2017**, 245-296		3
24	Novel theoretically designed HIV-1 non-nucleoside reverse transcriptase inhibitors derived from nevirapine. *Journal of Molecular Modeling*, **2014**, 20, 2451	2	3
23	Comparative study of Minnesota functionals performance on ferroelectric BaTiO3 and PbTiO3. *Physical Review Materials*, **2020**, 4,	3.2	3
22	Quantum calculation of protein NMR chemical shifts based on the automated fragmentation method. *Advances in Experimental Medicine and Biology*, **2015**, 827, 49-70	3.6	3
21	Directional Proton Transfer in the Reaction of the Simplest Criegee Intermediate with Water Involving the Formation of Transient HO. *Journal of Physical Chemistry Letters*, **2021**, 12, 3379-3386	6.4	3
20	Drug-guided screening for pancreatic lipase inhibitors in functional foods. *Food and Function*, **2021**, 12, 4644-4653	6.1	3
19	Phase Transition of Ice at High Pressures and Low Temperatures. *Molecules*, **2020**, 25,	4.8	2
18	Cholesterylation of Smoothened is a calcium-accelerated autoreaction involving an intramolecular ester intermediate.. *Cell Research*, **2022**,	24.7	2
17	Investigating mechanism of sweetness intensity differences through dynamic analysis of sweetener-T1R2-membrane systems.. *Food Chemistry*, **2021**, 374, 131807	8.5	2
16	Ultrasensitive Sensing of Volatile Organic Compounds Using a Cu-Doped SnO2-NiO p-n Heterostructure That Shows Significant Raman Enhancement**. *Angewandte Chemie*, **2021**, 133, 26464	3.6	2
15	Development of a New Scoring Function for Virtual Screening: APBScore. *Journal of Chemical Information and Modeling*, **2020**, 60, 6355-6365	6.1	2
14	Ab initio determination of crystal stability of di-p-tolyl disulfide. *Scientific Reports*, **2021**, 11, 7076	4.9	2

13	Accurate Prediction of Absorption Spectral Shifts of Proteorhodopsin Using a Fragment-Based Quantum Mechanical Method. *Molecules*, **2021**, 26,	4.8	2
12	Accurate Calculation of Electric Fields Inside Enzymes. *Methods in Enzymology*, **2016**, 578, 45-72	1.7	2
11	Predicted PAR1 inhibitors from multiple computational methods. *Chemical Physics Letters*, **2016**, 659, 295-303	2.5	2
10	COMPUTATIONAL STUDY OF HIV-1 gp41 NHR TRIMER: INHIBITION MECHANISMS OF N-SUBSTITUTED PYRROLE DERIVATIVES AND FRAGMENT-BASED VIRTUAL SCREENING. *Journal of Theoretical and Computational Chemistry*, **2013**, 12, 1341001	1.8	1
9	Computational Analysis of Residue-Specific Binding Free Energies of Androgen Receptor to Ligands. *Frontiers in Molecular Biosciences*, **2021**, 8, 646524	5.6	1
8	Glucose-Lipopeptide Conjugates Reveal the Role of Glucose Modification Position in Complexation and the Potential of Malignant Melanoma Therapy. *Journal of Medicinal Chemistry*, **2021**, 64, 11483-11495	8.3	1
7	Automated fragmentation quantum mechanical calculation of C and H chemical shifts in molecular crystals. *Journal of Chemical Physics*, **2021**, 154, 064502	3.9	0
6	Discovering inhibitors of TEAD palmitate binding pocket through virtual screening and molecular dynamics simulation.. *Computational Biology and Chemistry*, **2022**, 98, 107648	3.6	0
5	Fragment-Based Quantum Mechanical Calculation of Excited-State Properties of Fluorescent RNAs.. *Frontiers in Chemistry*, **2021**, 9, 801062	5	0
4	Crius: A novel fragment-based algorithm of de novo substrate prediction for enzymes. *Protein Science*, **2018**, 27, 1526-1534	6.3	
3	QM Implementation in Drug Design: Does It Really Help?. *Methods in Molecular Biology*, **2020**, 2114, 19-35	1.4	
2	Analysis of the binding modes of the first- and second-generation antiandrogens with respect to F876L mutation. *Chemical Biology and Drug Design*, **2021**, 98, 60-72	2.9	
1	A fixed multi-site interaction charge model for an accurate prediction of the QM/MM interactions. *Physical Chemistry Chemical Physics*, **2021**, 23, 21001-21012	3.6	