

# Yifei Qi

## List of Publications by Year in descending order

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254  
papers

15,318  
citations

36303

51  
h-index

23533

111  
g-index

258  
all docs

258  
docs citations

258  
times ranked

13175  
citing authors

#	ARTICLE	IF	CITATIONS
1	CHARMM-GUI Input Generator for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations Using the CHARMM36 Additive Force Field. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 405-413.	5.3	2,567
2	CHARMM-GUI Membrane Builder toward realistic biological membrane simulations. <i>Journal of Computational Chemistry</i> , 2014, 35, 1997-2004.	3.3	1,802
3	End-Point Binding Free Energy Calculation with MM/PBSA and MM/GBSA: Strategies and Applications in Drug Design. <i>Chemical Reviews</i> , 2019, 119, 9478-9508.	47.7	1,064
4	Full-dimensional time-dependent treatment for diatomic reactions: The H <sub>2</sub> +OH reaction. <i>Journal of Chemical Physics</i> , 1994, 101, 1146-1156.	3.0	422
5	CHARMM-GUI Membrane Builder for Complex Biological Membrane Simulations with Glycolipids and Lipoglycans. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 775-786.	5.3	388
6	CHARMM-GUI Martini Maker for Coarse-Grained Simulations with the Martini Force Field. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4486-4494.	5.3	340
7	Interaction Entropy: A New Paradigm for Highly Efficient and Reliable Computation of Protein-Ligand Binding Free Energy. <i>Journal of the American Chemical Society</i> , 2016, 138, 5722-5728.	13.7	297
8	Quantum reactive scattering with a deep well: Time-dependent calculation for H+O <sub>2</sub> reaction and bound state characterization for HO <sub>2</sub> . <i>Journal of Chemical Physics</i> , 1994, 101, 3671-3678.	3.0	265
9	Assessing the performance of MM/PBSA and MM/GBSA methods. 7. Entropy effects on the performance of end-point binding free energy calculation approaches. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 14450-14460.	2.8	243
10	CHARMM-GUI 10 years for biomolecular modeling and simulation. <i>Journal of Computational Chemistry</i> , 2017, 38, 1114-1124.	3.3	224
11	CHARMM-GUI Glycan Modeler for modeling and simulation of carbohydrates and glycoconjugates. <i>Glycobiology</i> , 2019, 29, 320-331.	2.5	222
12	CHARMM-GUI PDB Manipulator for Advanced Modeling and Simulations of Proteins Containing Nonstandard Residues. <i>Advances in Protein Chemistry and Structural Biology</i> , 2014, 96, 235-265.	2.3	214
13	Effects of N-glycosylation on protein conformation and dynamics: Protein Data Bank analysis and molecular dynamics simulation study. <i>Scientific Reports</i> , 2015, 5, 8926.	3.3	187
14	Accurate quantum calculation for the benchmark reaction H <sub>2</sub> +OH <sup>+</sup> H <sub>2</sub> O +H in five-dimensional space: Reaction probabilities for J=0. <i>Journal of Chemical Physics</i> , 1993, 99, 5615-5618.	3.0	175
15	Developing Polarized Protein-Specific Charges for Protein Dynamics: MD Free Energy Calculation of pKa Shifts for Asp26/Asp20 in Thioredoxin. <i>Biophysical Journal</i> , 2008, 95, 1080-1088.	0.5	151
16	CHARMM-GUI Martini Maker for modeling and simulation of complex bacterial membranes with lipopolysaccharides. <i>Journal of Computational Chemistry</i> , 2017, 38, 2354-2363.	3.3	150
17	DeepDDG: Predicting the Stability Change of Protein Point Mutations Using Neural Networks. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 1508-1514.	5.4	146
18	Exact full-dimensional bound state calculations for (HF) <sub>2</sub> , (DF) <sub>2</sub> , and HFDF. <i>Journal of Chemical Physics</i> , 1995, 102, 2315-2325.	3.0	132

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19	Effect of mutations on binding of ligands to guanine riboswitch probed by free energy perturbation and molecular dynamics simulations. <i>Nucleic Acids Research</i> , 2019, 47, 6618-6631.	14.5	130
20	LLPSDB: a database of proteins undergoing liquid-liquid phase separation in vitro. <i>Nucleic Acids Research</i> , 2020, 48, D320-D327.	14.5	130
21	Development of Accurate Quantum Dynamical Methods for Tetraatomic Reactions. <i>Journal of Physical Chemistry A</i> , 1997, 101, 2746-2754.	2.5	128
22	Accurate quantum calculations for $H_2+OH^{\ddagger}H_2O+H$ : Reaction probabilities, cross sections, and rate constants. <i>Journal of Chemical Physics</i> , 1994, 100, 2697-2706.	3.0	120
23	Quantum adsorption dynamics of a diatomic molecule on surface: Four-dimensional fixed-site model for $H_2$ on $Cu(111)$ . <i>Journal of Chemical Physics</i> , 1995, 102, 6280-6289.	3.0	117
24	New Advance in Computational Chemistry: Full Quantum Mechanical ab Initio Computation of Streptavidin-Biotin Interaction Energy. <i>Journal of Physical Chemistry B</i> , 2003, 107, 12039-12041.	2.6	117
25	A reactant-product decoupling method for state-to-state reactive scattering. <i>Journal of Chemical Physics</i> , 1996, 105, 6072-6074.	3.0	114
26	Computational Protein Design with Deep Learning Neural Networks. <i>Scientific Reports</i> , 2018, 8, 6349.	3.3	112
27	Time-Dependent Wave Packet Approach to State-to-State Reactive Scattering and Application to $H + O_2$ Reaction. <i>The Journal of Physical Chemistry</i> , 1996, 100, 6898-6903.	2.9	111
28	Complex reaction processes in combustion unraveled by neural network-based molecular dynamics simulation. <i>Nature Communications</i> , 2020, 11, 5713.	12.8	111
29	Quantum calculations of reaction probabilities for $HO + CO^{\ddagger} H + CO_2$ and bound states of HOCO. <i>Journal of Chemical Physics</i> , 1995, 103, 6512-6519.	3.0	107
30	Hydrogen-bond structure dynamics in bulk water: insights from <i>ab initio</i> simulations with coupled cluster theory. <i>Chemical Science</i> , 2018, 9, 2065-2073.	7.4	98
31	Interaction entropy for protein-protein binding. <i>Journal of Chemical Physics</i> , 2017, 146, 124124.	3.0	92
32	CHARMM-GUI HMMM Builder for Membrane Simulations with the Highly Mobile Membrane-Mimetic Model. <i>Biophysical Journal</i> , 2015, 109, 2012-2022.	0.5	89
33	An accurate free energy estimator: based on MM/PBSA combined with interaction entropy for protein-ligand binding affinity. <i>Nanoscale</i> , 2020, 12, 10737-10750.	5.6	88
34	An Electrochemical Biosensor with Dual Signal Outputs: Toward Simultaneous Quantification of pH and $O_2$ in the Brain upon Ischemia and in a Tumor during Cancer Starvation Therapy. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 10471-10475.	13.8	84
35	Interaction Entropy for Computational Alanine Scanning. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 1112-1122.	5.4	80
36	MolGpka: A Web Server for Small Molecule $pK_a$ Prediction Using a Graph-Convolutional Neural Network. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3159-3165.	5.4	79

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37	Calculations of Solvation Free Energy through Energy Reweighting from Molecular Mechanics to Quantum Mechanics. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 499-511.	5.3	78
38	Computational Alanine Scanning with Interaction Entropy for Protein-Ligand Binding Free Energies. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1772-1780.	5.3	78
39	Automated Fragmentation QM/MM Calculation of Amide Proton Chemical Shifts in Proteins with Explicit Solvent Model. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2104-2114.	5.3	73
40	Six-dimensional quantum calculations of vibration-rotation-tunneling levels of $\hat{1}/21$ and $\hat{1}/22$ HCl-stretching excited (HCl) <sub>2</sub> . <i>Journal of Chemical Physics</i> , 1998, 108, 4804-4816.	3.0	66
41	BamA POTRA Domain Interacts with a Native Lipid Membrane Surface. <i>Biophysical Journal</i> , 2016, 110, 2698-2709.	0.5	65
42	Photofragmentation of HF dimer: Quantum dynamics studies on ab initio potential energy surfaces. <i>Journal of Chemical Physics</i> , 1993, 99, 6624-6633.	3.0	64
43	Symmetry and rotational orientation effects in dissociative adsorption of diatomic molecules on metals: H <sub>2</sub> and HD on Cu(111). <i>Journal of Chemical Physics</i> , 1994, 101, 1555-1563.	3.0	64
44	Dynamics and Interactions of OmpF and LPS: Influence on Pore Accessibility and Ion Permeability. <i>Biophysical Journal</i> , 2016, 110, 930-938.	0.5	64
45	Time-dependent quantum dynamics study of the Cl+H <sub>2</sub> reaction. <i>Journal of Chemical Physics</i> , 2000, 113, 1434-1440.	3.0	60
46	Quantum Fragment Based <i>ab Initio</i> Molecular Dynamics for Proteins. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5897-5905.	5.3	59
47	CHARMM-GUI Supports Hydrogen Mass Repartitioning and Different Protonation States of Phosphates in Lipopolysaccharides. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 831-839.	5.4	59
48	Accelerated Molecular Dynamics Simulation for Helical Proteins Folding in Explicit Water. <i>Frontiers in Chemistry</i> , 2019, 7, 540.	3.6	56
49	A time-dependent approach to flux calculation in molecular photofragmentation: Vibrational predissociation of HF-DF. <i>Journal of Chemical Physics</i> , 1995, 102, 124-132.	3.0	55
50	Fragment Quantum Mechanical Method for Large-Sized Ion-Water Clusters. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2021-2034.	5.3	54
51	Use of negative complex potential as absorbing potential. <i>Journal of Chemical Physics</i> , 1998, 108, 1429-1433.	3.0	52
52	Time-dependent quantum wave packet studies of the F+HCl and F+DCI reactions. <i>Journal of Chemical Physics</i> , 2000, 113, 10105-10113.	3.0	52
53	Quantum computational analysis for drug resistance of HIV-1 reverse transcriptase to nevirapine through point mutations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 61, 423-432.	2.6	52
54	Quantum dynamics studies of adsorption and desorption of hydrogen at a Cu(111) surface. <i>Journal of Chemical Physics</i> , 1993, 99, 1373-1381.	3.0	51

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55	Proteinâ€“Ligand Empirical Interaction Components for Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 1793-1806.	5.4	51
56	Interaction entropy for computational alanine scanning in protein-protein binding. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2018, 8, e1342.	14.6	51
57	Maturation Mechanism of Severe Acute Respiratory Syndrome (SARS) Coronavirus 3C-like Proteinase. <i>Journal of Biological Chemistry</i> , 2010, 285, 28134-28140.	3.4	50
58	Dissociative chemisorption of H <sub>2</sub> on Ni surface: Timeâ€“dependent quantum dynamics calculation and comparison with experiment. <i>Journal of Chemical Physics</i> , 1992, 96, 3866-3874.	3.0	49
59	Reactant-product decoupling method for state-to-state reactive scattering: A case study for 3D H+H <sub>2</sub> exchange reaction (j=0). <i>Journal of Chemical Physics</i> , 1997, 106, 1742-1748.	3.0	49
60	Timeâ€“dependent treatment of vibrational predissociation within the golden rule approximation. <i>Journal of Chemical Physics</i> , 1991, 95, 6449-6455.	3.0	47
61	CHARMM-GUI PACE CG Builder for Solution, Micelle, and Bilayer Coarse-Grained Simulations. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 1003-1009.	5.4	47
62	Calculation of proteinâ€“ligand binding affinities based on a fragment quantum mechanical method. <i>RSC Advances</i> , 2015, 5, 107020-107030.	3.6	47
63	DenseCPD: Improving the Accuracy of Neural-Network-Based Computational Protein Sequence Design with DenseNet. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1245-1252.	5.4	47
64	Identifying Allosteric Binding Sites in Proteins with a Two-State Goâ€“Model for Novel Allosteric Effector Discovery. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2962-2971.	5.3	46
65	DFT Calculations on the Mechanism of Transition-Metal-Catalyzed Reaction of Diazo Compounds with Phenols: Oâ€“H Insertion versus Câ€“H Insertion. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6485-6492.	2.5	45
66	Single Biosensor for Simultaneous Quantification of Glucose and pH in a Rat Brain of Diabetic Model Using Both Current and Potential Outputs. <i>Analytical Chemistry</i> , 2017, 89, 6656-6662.	6.5	45
67	Quantum dynamics study of Li + HF reaction. <i>Theoretical Chemistry Accounts</i> , 1997, 96, 31-38.	1.4	44
68	A New Quantum Calibrated Force Field for Zincâ€“Protein Complex. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1788-1798.	5.3	44
69	The impact of interior dielectric constant and entropic change on HIV-1 complex binding free energy prediction. <i>Structural Dynamics</i> , 2018, 5, 064101.	2.3	44
70	DeepBSPâ€“a Machine Learning Method for Accurate Prediction of Proteinâ€“Ligand Docking Structures. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2231-2240.	5.4	44
71	Progress of basis optimization techniques in variational calculation of quantum reactive scattering. <i>Journal of Chemical Physics</i> , 1991, 94, 6047-6054.	3.0	43
72	6D quantum calculation of energy levels for HF stretching excited (HF) <sub>2</sub> . <i>Journal of Chemical Physics</i> , 1995, 103, 2548-2554.	3.0	42

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73	A numerically stable restrained electrostatic potential charge fitting method. <i>Journal of Computational Chemistry</i> , 2013, 34, 847-853.	3.3	42
74	Modeling and simulation of bacterial outer membranes and interactions with membrane proteins. <i>Current Opinion in Structural Biology</i> , 2017, 43, 131-140.	5.7	42
75	CHARMMâ€GLUI <i>&lt;i&gt;Nanodisc Builder&lt;/i&gt;</i> for modeling and simulation of various nanodisc systems. <i>Journal of Computational Chemistry</i> , 2019, 40, 893-899.	3.3	42
76	Application of Semirigid Vibrating Rotor Target Model to the Reaction of O(3P) + CH4â†' CH3+ OHâ€. <i>Journal of Physical Chemistry A</i> , 2001, 105, 2530-2534.	2.5	41
77	A timeâ€dependent golden rule wave packet calculation for vibrational predissociation of D2HF. <i>Journal of Chemical Physics</i> , 1992, 97, 927-934.	3.0	40
78	Timeâ€dependent spectral calculation of bound and resonance energies of HO2. <i>Journal of Chemical Physics</i> , 1996, 104, 3664-3671.	3.0	40
79	Unfolding of a ClC chloride transporter retains memory of its evolutionary history. <i>Nature Chemical Biology</i> , 2018, 14, 489-496.	8.0	39
80	Preferred Orientations of Phosphoinositides in Bilayers and Their Implications in Protein Recognition Mechanisms. <i>Journal of Physical Chemistry B</i> , 2014, 118, 4315-4325.	2.6	38
81	Electronic Polarization Is Important in Stabilizing the Native Structures of Proteins. <i>Journal of Physical Chemistry B</i> , 2009, 113, 16059-16064.	2.6	37
82	Accurate and Efficient Calculation of Proteinâ€Protein Binding Free Energy-Interaction Entropy with Residue Type-Specific Dielectric Constants. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 272-281.	5.4	37
83	Quantum mechanical calculation for photodissociation of hydrogen peroxide. <i>Journal of Chemical Physics</i> , 1993, 98, 6276-6283.	3.0	35
84	A timeâ€dependent calculation for vibrational predissociation of H2HF. <i>Journal of Chemical Physics</i> , 1992, 97, 3149-3156.	3.0	34
85	Preferred conformations of <i>&lt;i&gt;N&lt;/i&gt;</i> -glycan core pentasaccharide in solution and in glycoproteins. <i>Glycobiology</i> , 2016, 26, cwv083.	2.5	34
86	HobPre: accurate prediction of human oral bioavailability for small molecules. <i>Journal of Cheminformatics</i> , 2022, 14, 1.	6.1	32
87	Hybrid QM/MM study of FMO complex with polarized protein-specific charge. <i>Scientific Reports</i> , 2015, 5, 17096.	3.3	30
88	Mechanistic Investigation of Aromatic C(sp<sup>2</sup>)â€H and Alkyl C(sp<sup>3</sup>)â€H Bond Insertion by Gold Carbenes. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1925-1932.	2.5	29
89	Decoding molecular mechanism of inhibitor bindings to CDK2 using molecular dynamics simulations and binding free energy calculations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 985-996.	3.5	29
90	The origin of the cooperativity in the streptavidin-biotin system: A computational investigation through molecular dynamics simulations. <i>Scientific Reports</i> , 2016, 6, 27190.	3.3	28

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91	Quantum dynamical studies for photodissociation of H <sub>2</sub> O <sub>2</sub> at 248 and 266 nm. <i>Journal of Chemical Physics</i> , 1994, 100, 5631-5638.	3.0	27
92	Quantum dynamics study of the Cl+D <sub>2</sub> reaction: Time-dependent wave packet calculations. <i>Journal of Chemical Physics</i> , 2000, 113, 7182-7187.	3.0	27
93	Time-dependent quantum wave packet study of the C+CH reaction. <i>Journal of Chemical Physics</i> , 2001, 115, 731-738.	3.0	27
94	A mixed quantum-classical semirigid vibrating rotor target approach to methane dissociation on Ni surface. <i>Journal of Chemical Physics</i> , 2003, 118, 8954-8959.	3.0	27
95	Accurate quantum mechanical calculation for the N+OH reaction. <i>Journal of Chemical Physics</i> , 2003, 118, 6852-6857.	3.0	27
96	An algebraic variational approach to dissociative adsorption of a diatomic molecule on a smooth metal surface. <i>Journal of Chemical Physics</i> , 1992, 97, 6784-6791.	3.0	26
97	Energy Dependence of State-to-State Reaction Probabilities for H <sub>2</sub> + OH → H + H <sub>2</sub> O in Six Dimensions. <i>The Journal of Physical Chemistry</i> , 1996, 100, 13901-13903.	2.9	26
98	Full quantum mechanical study of binding of HIV-1 protease drugs. <i>International Journal of Quantum Chemistry</i> , 2005, 103, 246-257.	2.0	26
99	Anchor-Locker Binding Mechanism of the Coronavirus Spike Protein to Human ACE2: Insights from Computational Analysis. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3529-3542.	5.4	26
100	Discovery of Novel Allosteric Effectors Based on the Predicted Allosteric Sites for Escherichia coli D-3-Phosphoglycerate Dehydrogenase. <i>PLoS ONE</i> , 2014, 9, e94829.	2.5	26
101	HergSPred: Accurate Classification of hERG Blockers/Nonblockers with Machine-Learning Models. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 1830-1839.	5.4	26
102	Vibrational predissociation of HF dimer in $\hat{1}/2$ HF=1: Influence of initially excited intermolecular vibrations on the fragmentation dynamics. <i>Journal of Chemical Physics</i> , 1995, 102, 4382-4389.	3.0	25
103	CHARMM-GUI MDFF/xMDFF Utilizer for Molecular Dynamics Flexible Fitting Simulations in Various Environments. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3718-3723.	2.6	24
104	Molecular Dynamics Simulation of Zinc Ion in Water with an ab Initio Based Neural Network Potential. <i>Journal of Physical Chemistry A</i> , 2019, 123, 6587-6595.	2.5	24
105	Total and partial decay widths in vibrational predissociation of HF dimer. <i>Journal of Chemical Physics</i> , 1993, 98, 5978-5981.	3.0	23
106	Computational analysis of hot spots and binding mechanism in the PD-1/PD-L1 interaction. <i>RSC Advances</i> , 2019, 9, 14944-14956.	3.6	23
107	Thermodynamic Insights of Base Flipping in TNA Duplex: Force Fields, Salt Concentrations, and Free-Energy Simulation Methods. <i>CCS Chemistry</i> , 2021, 3, 1026-1039.	7.8	23
108	Theoretical model for the dynamics of hydrogen recombination on the Si(100) $\hat{\epsilon}$ (2Å-1) surface. <i>Journal of Chemical Physics</i> , 1992, 97, 596-604.	3.0	22

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109	A Coupled Ionization-Conformational Equilibrium Is Required To Understand the Properties of Ionizable Residues in the Hydrophobic Interior of Staphylococcal Nuclease. <i>Journal of the American Chemical Society</i> , 2018, 140, 1639-1648.	13.7	22
110	BAR-based optimum adaptive steered MD for configurational sampling. <i>Journal of Computational Chemistry</i> , 2019, 40, 1270-1289.	3.3	22
111	Understanding the selectivity of inhibitors toward PI4KIII <sup>1</sup> and PI4KIII <sup>2</sup> based molecular modeling. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 22103-22112.	2.8	22
112	Calculation of hot spots for protein-protein interaction in p53/PM1-MDM2/MDMX complexes. <i>Journal of Computational Chemistry</i> , 2019, 40, 1045-1056.	3.3	22
113	Studying the Effect of Site-Specific Hydrophobicity and Polarization on Hydrogen Bond Energy of Protein Using a Polarizable Method. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2157-2164.	5.3	21
114	Full QM Calculation of RNA Energy Using Electrostatically Embedded Generalized Molecular Fractionation with Conjugate Caps Method. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2503-2514.	2.5	21
115	Study of SHMT2 Inhibitors and Their Binding Mechanism by Computational Alanine Scanning. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3871-3878.	5.4	21
116	Sulfur-substitution-induced base flipping in the DNA duplex. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 14923-14940.	2.8	21
117	Entropic effect and residue specific entropic contribution to the cooperativity in streptavidin-biotin binding. <i>Nanoscale</i> , 2020, 12, 7134-7145.	5.6	21
118	Time-Dependent Quantum Dynamics Study of the Cl + HD Reaction. <i>Journal of Physical Chemistry A</i> , 2000, 104, 10517-10525.	2.5	20
119	Conformational Flexibility of a Short Loop near the Active Site of the SARS-3CL <sup>pro</sup> is Essential to Maintain Catalytic Activity. <i>Scientific Reports</i> , 2016, 6, 20918.	3.3	20
120	Effect of polarization on HIV-1 protease and fluoro-substituted inhibitors binding energies by large scale molecular dynamics simulations. <i>Scientific Reports</i> , 2017, 7, 42223.	3.3	20
121	An efficient method for computing excess free energy of liquid. <i>Science China Chemistry</i> , 2018, 61, 135-140.	8.2	20
122	Mechanistic Studies of CO <sub>2</sub> Cycloaddition Reaction Catalyzed by Amine-Functionalized Ionic Liquids. <i>Frontiers in Chemistry</i> , 2019, 7, 615.	3.6	20
123	Double-Well Ultra-Coarse-Grained Model to Describe Protein Conformational Transitions. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6678-6689.	5.3	20
124	Quantum mechanical tunneling through a time-dependent barrier. <i>Journal of Chemical Physics</i> , 1996, 105, 8628-8632.	3.0	19
125	Effect of interprotein polarization on protein-protein binding energy. <i>Journal of Computational Chemistry</i> , 2012, 33, 1416-1420.	3.3	19
126	Development of an Effective Polarizable Bond Method for Biomolecular Simulation. <i>Journal of Physical Chemistry B</i> , 2013, 117, 14885-14893.	2.6	19



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127	Constructing Optimal Coarse-Grained Sites of Huge Biomolecules by Fluctuation Maximization. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2091-2100.	5.3	19
128	An Electrochemical Biosensor with Dual Signal Outputs: Toward Simultaneous Quantification of pH and O <sub>2</sub> in the Brain upon Ischemia and in a Tumor during Cancer Starvation Therapy. <i>Angewandte Chemie</i> , 2017, 129, 10607-10611.	2.0	19
129	Probing the Ion-Specific Effects at the Water/Air Interface and Water-Mediated Ion Pairing in Sodium Halide Solution with <i>Ab Initio</i> Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2018, 122, 10202-10209.	2.6	19
130	CHARMM-GUI DEER facilitator for spin-pair distance distribution calculations and preparation of restrained-ensemble molecular dynamics simulations. <i>Journal of Computational Chemistry</i> , 2020, 41, 415-420.	3.3	19
131	Dissociative Adsorption of O <sub>2</sub> on Cu(110) and Cu(100): A Three-Dimensional Quantum Dynamics Studies. <i>The Journal of Physical Chemistry</i> , 1996, 100, 11432-11437.	2.9	18
132	Simulation of the thermodynamics of folding and unfolding of the Trp-cage mini-protein TC5b using different combinations of force fields and solvation models. <i>Science China Chemistry</i> , 2010, 53, 196-201.	8.2	18
133	Insight into Early-Stage Unfolding of GPI-Anchored Human Prion Protein. <i>Biophysical Journal</i> , 2015, 109, 2090-2100.	0.5	18
134	A new algorithm for construction of coarse-grained sites of large biomolecules. <i>Journal of Computational Chemistry</i> , 2016, 37, 795-804.	3.3	18
135	Effect of Substituents in Different Positions of Aminothiazole Hinge-Binding Scaffolds on Inhibitor-CDK2 Association Probed by Interaction Entropy Method. <i>ACS Omega</i> , 2018, 3, 18052-18064.	3.5	18
136	Allosteric sites can be identified based on the residue-residue interaction energy difference. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015, 83, 1375-1384.	2.6	17
137	A Fragment Quantum Mechanical Method for Metalloproteins. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1430-1439.	5.3	17
138	Residue-specific free energy analysis in ligand bindings to JAK2. <i>Molecular Physics</i> , 2018, 116, 2633-2641.	1.7	16
139	Binding modes and conformational changes of FK506-binding protein 51 induced by inhibitor bindings: insight into molecular mechanisms based on multiple simulation technologies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 2141-2155.	3.5	16
140	Roles of glycans in interactions between gp120 and HIV broadly neutralizing antibodies. <i>Glycobiology</i> , 2015, 26, cwv101.	2.5	15
141	Functional Loop Dynamics of the Streptavidin-Biotin Complex. <i>Scientific Reports</i> , 2015, 5, 7906.	3.3	15
142	Correct folding of an $\alpha$ -helix and a $\beta$ -hairpin using a polarized 2D torsional potential. <i>Scientific Reports</i> , 2015, 5, 10359.	3.3	15
143	A systematic study on RNA NMR chemical shift calculation based on the automated fragmentation QM/MM approach. <i>RSC Advances</i> , 2016, 6, 108590-108602.	3.6	14
144	Exploring the Reasons for Decrease in Binding Affinity of HIV-2 Against HIV-1 Protease Complex Using Interaction Entropy Under Polarized Force Field. <i>Frontiers in Chemistry</i> , 2018, 6, 380.	3.6	14

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