Yifei Qi

List of Publications by Citations

242 papers	9,657 citations	46 h-index	92 g-index
258 ext. papers	12,573 ext. citations	4.8 avg, IF	6.57 L-index

#	Paper	IF	Citations
242	CHARMM-GUI Input Generator for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations Using the CHARMM36 Additive Force Field. *Journal of Chemical Theory and Computation*, **2016**, 12, 405-13	6.4	1303
241	CHARMM-GUI Membrane Builder toward realistic biological membrane simulations. *Journal of Computational Chemistry*, **2014**, 35, 1997-2004	3.5	1004
240	End-Point Binding Free Energy Calculation with MM/PBSA and MM/GBSA: Strategies and Applications in Drug Design. *Chemical Reviews*, **2019**, 119, 9478-9508	68.1	449
239	Full-dimensional time-dependent treatment for diatom□diatom reactions: The H2+OH reaction. *Journal of Chemical Physics*, **1994**, 101, 1146-1156	3.9	378
238	Quantum reactive scattering with a deep well: Time-dependent calculation for H+O2 reaction and bound state characterization for HO2. *Journal of Chemical Physics*, **1994**, 101, 3671-3678	3.9	245
237	CHARMM-GUI Martini Maker for Coarse-Grained Simulations with the Martini Force Field. *Journal of Chemical Theory and Computation*, **2015**, 11, 4486-94	6.4	181
236	Interaction Entropy: A New Paradigm for Highly Efficient and Reliable Computation of Protein-Ligand Binding Free Energy. *Journal of the American Chemical Society*, **2016**, 138, 5722-8	16.4	178
235	Accurate quantum calculation for the benchmark reaction H2+OH→H2O +H in five-dimensional space: Reaction probabilities for J=0. *Journal of Chemical Physics*, **1993**, 99, 5615-5618	3.9	152
234	CHARMM-GUI Membrane Builder for Complex Biological Membrane Simulations with Glycolipids and Lipoglycans. *Journal of Chemical Theory and Computation*, **2019**, 15, 775-786	6.4	152
233	Assessing the performance of MM/PBSA and MM/GBSA methods. 7. Entropy effects on the performance of end-point binding free energy calculation approaches. *Physical Chemistry Chemical Physics*, **2018**, 20, 14450-14460	3.6	149
232	Developing polarized protein-specific charges for protein dynamics: MD free energy calculation of pKa shifts for Asp26/Asp20 in thioredoxin. *Biophysical Journal*, **2008**, 95, 1080-8	2.9	136
231	Effects of N-glycosylation on protein conformation and dynamics: Protein Data Bank analysis and molecular dynamics simulation study. *Scientific Reports*, **2015**, 5, 8926	4.9	122
230	Exact full-dimensional bound state calculations for (HF)2, (DF)2, and HFDF. *Journal of Chemical Physics*, **1995**, 102, 2315-2325	3.9	121
229	CHARMM-GUI 10 years for biomolecular modeling and simulation. *Journal of Computational Chemistry*, **2017**, 38, 1114-1124	3.5	119
228	Development of Accurate Quantum Dynamical Methods for Tetraatomic Reactions. *Journal of Physical Chemistry A*, **1997**, 101, 2746-2754	2.8	118
227	New Advance in Computational Chemistry: Full Quantum Mechanical ab Initio Computation of Streptavidin-Biotin Interaction Energy. *Journal of Physical Chemistry B*, **2003**, 107, 12039-41	3.4	111
226	Quantum adsorption dynamics of a diatomic molecule on surface: Four-dimensional fixed-site model for H2 on Cu(111). *Journal of Chemical Physics*, **1995**, 102, 6280-6289	3.9	109

225	Time-Dependent Wave Packet Approach to State-to-State Reactive Scattering and Application to H + O2 Reaction. *The Journal of Physical Chemistry*, **1996**, 100, 6898-6903		104
224	CHARMM-GUI Glycan Modeler for modeling and simulation of carbohydrates and glycoconjugates. *Glycobiology*, **2019**, 29, 320-331	5.8	101
223	A reactant-product decoupling method for state-to-state reactive scattering. *Journal of Chemical Physics*, **1996**, 105, 6072-6074	3.9	101
222	Accurate quantum calculations for H2+OH-H2O+H: Reaction probabilities, cross sections, and rate constants. *Journal of Chemical Physics*, **1994**, 100, 2697-2706	3.9	101
221	Quantum calculations of reaction probabilities for HO + CO-H + CO2 and bound states of HOCO. *Journal of Chemical Physics*, **1995**, 103, 6512-6519	3.9	97
220	CHARMM-GUI PDB manipulator for advanced modeling and simulations of proteins containing nonstandard residues. *Advances in Protein Chemistry and Structural Biology*, **2014**, 96, 235-65	5.3	96
219	Effect of mutations on binding of ligands to guanine riboswitch probed by free energy perturbation and molecular dynamics simulations. *Nucleic Acids Research*, **2019**, 47, 6618-6631	20.1	77
218	Computational Protein Design with Deep Learning Neural Networks. *Scientific Reports*, **2018**, 8, 6349	4.9	72
217	Calculations of Solvation Free Energy through Energy Reweighting from Molecular Mechanics to Quantum Mechanics. *Journal of Chemical Theory and Computation*, **2016**, 12, 499-511	6.4	70
216	Hydrogen-bond structure dynamics in bulk water: insights from simulations with coupled cluster theory. *Chemical Science*, **2018**, 9, 2065-2073	9.4	68
215	Interaction entropy for protein-protein binding. *Journal of Chemical Physics*, **2017**, 146, 124124	3.9	65
214	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
213	LLPSDB: a database of proteins undergoing liquid-liquid phase separation in vitro. *Nucleic Acids Research*, **2020**, 48, D320-D327	20.1	63
212	DeepDDG: Predicting the Stability Change of Protein Point Mutations Using Neural Networks. *Journal of Chemical Information and Modeling*, **2019**, 59, 1508-1514	6.1	62
211	Six-dimensional quantum calculations of vibration-rotation-tunneling levels of □1 and □2 HCl-stretching excited (HCl)2. *Journal of Chemical Physics*, **1998**, 108, 4804-4816	3.9	61
210	An Electrochemical Biosensor with Dual Signal Outputs: Toward Simultaneous Quantification of pH and O in the Brain upon Ischemia and in a Tumor during Cancer Starvation Therapy. *Angewandte Chemie - International Edition*, **2017**, 56, 10471-10475	16.4	60
209	CHARMM-GUI HMMM Builder for Membrane Simulations with the Highly Mobile Membrane-Mimetic Model. *Biophysical Journal*, **2015**, 109, 2012-22	2.9	60
208	Symmetry and rotational orientation effects in dissociative adsorption of diatomic molecules on metals: H2 and HD on Cu(111). *Journal of Chemical Physics*, **1994**, 101, 1555-1563	3.9	59

207	Photofragmentation of HF dimer: Quantum dynamics studies on ab initio potential energy surfaces. *Journal of Chemical Physics*, **1993**, 99, 6624-6633	3.9	58
206	Time-dependent quantum dynamics study of the Cl+H2 reaction. *Journal of Chemical Physics*, **2000**, 113, 1434-1440	3.9	56
205	Interaction Entropy for Computational Alanine Scanning. *Journal of Chemical Information and Modeling*, **2017**, 57, 1112-1122	6.1	55
204	Dynamics and Interactions of OmpF and LPS: Influence on Pore Accessibility and Ion Permeability. *Biophysical Journal*, **2016**, 110, 930-8	2.9	54
203	BamA POTRA Domain Interacts with a Native Lipid Membrane Surface. *Biophysical Journal*, **2016**, 110, 2698-2709	2.9	52
202	A time-dependent approach to flux calculation in molecular photofragmentation: Vibrational predissociation of HFDF. *Journal of Chemical Physics*, **1995**, 102, 124-132	3.9	50
201	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
200	An accurate free energy estimator: based on MM/PBSA combined with interaction entropy for protein-ligand binding affinity. *Nanoscale*, **2020**, 12, 10737-10750	7.7	49
199	Time-dependent quantum wave packet studies of the F+HCl and F+DCl reactions. *Journal of Chemical Physics*, **2000**, 113, 10105-10113	3.9	48
198	Use of negative complex potential as absorbing potential. *Journal of Chemical Physics*, **1998**, 108, 1429-1433	3.9	48
197	Quantum dynamics studies of adsorption and desorption of hydrogen at a Cu(111) surface. *Journal of Chemical Physics*, **1993**, 99, 1373-1381	3.9	46
196	Dissociative chemisorption of H2 on Ni surface: Time-dependent quantum dynamics calculation and comparison with experiment. *Journal of Chemical Physics*, **1992**, 96, 3866-3874	3.9	45
195	Computational Alanine Scanning with Interaction Entropy for Protein-Ligand Binding Free Energies. *Journal of Chemical Theory and Computation*, **2018**, 14, 1772-1780	6.4	44
194	Time-dependent treatment of vibrational predissociation within the golden rule approximation. *Journal of Chemical Physics*, **1991**, 95, 6449-6455	3.9	44
193	Quantum Fragment Based ab Initio Molecular Dynamics for Proteins. *Journal of Chemical Theory and Computation*, **2015**, 11, 5897-905	6.4	43
192	Complex reaction processes in combustion unraveled by neural network-based molecular dynamics simulation. *Nature Communications*, **2020**, 11, 5713	17.4	43
191	Identifying Allosteric Binding Sites in Proteins with a Two-State Go Model for Novel Allosteric Effector Discovery. *Journal of Chemical Theory and Computation*, **2012**, 8, 2962-71	6.4	42
190	Reactant-product decoupling method for state-to-state reactive scattering: A case study for 3D H+H2 exchange reaction (J=0). *Journal of Chemical Physics*, **1997**, 106, 1742-1748	3.9	42

189	Quantum dynamics study of Li + HF reaction. *Theoretical Chemistry Accounts*, **1997**, 96, 31-38	1.9	41
188	Application of Semirigid Vibrating Rotor Target Model to the Reaction of O(3P) + CH4 -> CH3 + OH. *Journal of Physical Chemistry A*, **2001**, 105, 2530-2534	2.8	40
187	Fragment Quantum Mechanical Method for Large-Sized Ion-Water Clusters. *Journal of Chemical Theory and Computation*, **2017**, 13, 2021-2034	6.4	39
186	A New Quantum Calibrated Force Field for Zinc-Protein Complex. *Journal of Chemical Theory and Computation*, **2013**, 9, 1788-98	6.4	38
185	Maturation mechanism of severe acute respiratory syndrome (SARS) coronavirus 3C-like proteinase. *Journal of Biological Chemistry*, **2010**, 285, 28134-40	5.4	38
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179	Interaction entropy for computational alanine scanning in protein–protein binding. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1342	7.9	34
178	A numerically stable restrained electrostatic potential charge fitting method. *Journal of Computational Chemistry*, **2013**, 34, 847-53	3.5	34
177	A time-dependent golden rule wave packet calculation for vibrational predissociation of D2HF. *Journal of Chemical Physics*, **1992**, 97, 927-934	3.9	34
176	Accelerated Molecular Dynamics Simulation for Helical Proteins Folding in Explicit Water. *Frontiers in Chemistry*, **2019**, 7, 540	5	33
175	CHARMM-GUI PACE CG Builder for solution, micelle, and bilayer coarse-grained simulations. *Journal of Chemical Information and Modeling*, **2014**, 54, 1003-9	6.1	33
174	Electronic polarization is important in stabilizing the native structures of proteins. *Journal of Physical Chemistry B*, **2009**, 113, 16059-64	3.4	33
173	DFT Calculations on the Mechanism of Transition-Metal-Catalyzed Reaction of Diazo Compounds with Phenols: O-H Insertion versus C-H Insertion. *Journal of Physical Chemistry A*, **2016**, 120, 6485-92	2.8	33
172	Calculation of protein–ligand binding affinities based on a fragment quantum mechanical method. *RSC Advances*, **2015**, 5, 107020-107030	3.7	32

171	Modeling and simulation of bacterial outer membranes and interactions with membrane proteins. *Current Opinion in Structural Biology*, **2017**, 43, 131-140	8.1	30
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168	The impact of interior dielectric constant and entropic change on HIV-1 complex binding free energy prediction. *Structural Dynamics*, **2018**, 5, 064101	3.2	29
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155	Mechanistic Investigation of Aromatic C(sp(2))-H and Alkyl C(sp(3))-H Bond Insertion by Gold Carbenes. *Journal of Physical Chemistry A*, **2016**, 120, 1925-32	2.8	23
154	An algebraic variational approach to dissociative adsorption of a diatomic molecule on a smooth metal surface. *Journal of Chemical Physics*, **1992**, 97, 6784-6791	3.9	23

153	Unfolding of a ClC chloride transporter retains memory of its evolutionary history. *Nature Chemical Biology*, **2018**, 14, 489-496	11.7	22
152	Total and partial decay widths in vibrational predissociation of HF dimer. *Journal of Chemical Physics*, **1993**, 98, 5978-5981	3.9	22
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150	Preferred orientations of phosphoinositides in bilayers and their implications in protein recognition mechanisms. *Journal of Physical Chemistry B*, **2014**, 118, 4315-25	3.4	21
149	The origin of the cooperativity in the streptavidin-biotin system: A computational investigation through molecular dynamics simulations. *Scientific Reports*, **2016**, 6, 27190	4.9	20
148	Decoding molecular mechanism of inhibitor bindings to CDK2 using molecular dynamics simulations and binding free energy calculations. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 985-996	3.6	20
147	Studying the Effect of Site-Specific Hydrophobicity and Polarization on Hydrogen Bond Energy of Protein Using a Polarizable Method. *Journal of Chemical Theory and Computation*, **2012**, 8, 2157-64	6.4	19
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139	Quantum mechanical tunneling through a time-dependent barrier. *Journal of Chemical Physics*, **1996**, 105, 8628-8632	3.9	17
138	Calculation of hot spots for protein-protein interaction in p53/PMI-MDM2/MDMX complexes. *Journal of Computational Chemistry*, **2019**, 40, 1045-1056	3.5	17
137	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
136	Computational analysis of hot spots and binding mechanism in the PD-1/PD-L1 interaction.. *RSC Advances*, **2019**, 9, 14944-14956	3.7	16

135	Entropic effect and residue specific entropic contribution to the cooperativity in streptavidin-biotin binding. *Nanoscale*, **2020**, 12, 7134-7145	7.7	16
134	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
133	Molecular Dynamics Simulation of Zinc Ion in Water with an ab Initio Based Neural Network Potential. *Journal of Physical Chemistry A*, **2019**, 123, 6587-6595	2.8	16
132	Sulfur-substitution-induced base flipping in the DNA duplex. *Physical Chemistry Chemical Physics*, **2019**, 21, 14923-14940	3.6	15
131	Dissociative Adsorption of O2on Cu(110) and Cu(100):Three-Dimensional Quantum Dynamics Studies. *The Journal of Physical Chemistry*, **1996**, 100, 11432-11437		15
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127	Simulation of the thermodynamics of folding and unfolding of the Trp-cage mini-protein TC5b using different combinations of force fields and solvation models. *Science China Chemistry*, **2010**, 53, 196-201	7.9	14
126	CHARMM-GUI MDFF/xMDFF Utilizer for Molecular Dynamics Flexible Fitting Simulations in Various Environments. *Journal of Physical Chemistry B*, **2017**, 121, 3718-3723	3.4	13
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123	Roles of glycans in interactions between gp120 and HIV broadly neutralizing antibodies. *Glycobiology*, **2016**, 26, 251-60	5.8	13
122	Folding simulations of a de novo designed protein with a betaalphabeta fold. *Biophysical Journal*, **2010**, 98, 321-9	2.9	13
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119	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
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115	Replacing Arginine 33 for Alanine in the Hemophore HasA from Pseudomonas aeruginosa Causes Closure of the H32 Loop in the Apo-Protein. *Biochemistry*, **2016**, 55, 2622-31	3.2	12
114	Effect of Substituents in Different Positions of Aminothiazole Hinge-Binding Scaffolds on Inhibitor□CDK2 Association Probed by Interaction Entropy Method. *ACS Omega*, **2018**, 3, 18052-18064	3.9	12
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93	Solid-State NMR-Restrained Ensemble Dynamics of a Membrane Protein in Explicit Membranes. *Biophysical Journal*, **2015**, 108, 1954-62	2.9	9
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89	Folding and thermodynamic studies of Trp-cage based on polarized force field. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	9
88	Quantification of Drive-Response Relationships Between Residues During Protein Folding. *Journal of Chemical Theory and Computation*, **2013**, 9,	6.4	9
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83	Computational analysis for residue-specific CDK2-inhibitor bindings *Chinese Journal of Chemical Physics*, **2019**, 32, 134-142	0.9	8
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