Pengfei Li

List of Publications by Year
in descending order

26 papers	2,674 citations	471477 17 h-index	526264 27 g-index
28 all docs	28 docs citations	28 times ranked	3436 citing authors

#	Article	IF	Citations
1	Rational Design of Particle Mesh Ewald Compatible Lennard-Jones Parameters for +2 Metal Cations in Explicit Solvent. Journal of Chemical Theory and Computation, 2013, 9, 2733-2748.	5.3	559
2	MCPB.py: A Python Based Metal Center Parameter Builder. Journal of Chemical Information and Modeling, 2016, 56, 599-604.	5.4	416
3	Systematic Parameterization of Monovalent Ions Employing the Nonbonded Model. Journal of Chemical Theory and Computation, 2015, 11, 1645-1657.	5.3	334
4	Taking into Account the Ion-Induced Dipole Interaction in the Nonbonded Model of Ions. Journal of Chemical Theory and Computation, 2014, 10, 289-297.	5.3	305
5	Metal Ion Modeling Using Classical Mechanics. Chemical Reviews, 2017, 117, 1564-1686.	47.7	266
6	Parameterization of Highly Charged Metal Ions Using the 12-6-4 LJ-Type Nonbonded Model in Explicit Water. Journal of Physical Chemistry B, 2015, 119, 883-895.	2.6	237
7	QM/MM Studies into the H₂O₂-Dependent Activity of Lytic Polysaccharide Monooxygenases: Evidence for the Formation of a Caged Hydroxyl Radical Intermediate. ACS Catalysis, 2018, 8, 1346-1351.	11.2	117
8	Parameterization of Monovalent Ions for the OPC3, OPC, TIP3P-FB, and TIP4P-FB Water Models. Journal of Chemical Information and Modeling, 2021, 61, 869-880.	5.4	81
9	Systematic Parametrization of Divalent Metal Ions for the OPC3, OPC, TIP3P-FB, and TIP4P-FB Water Models. Journal of Chemical Theory and Computation, 2020, 16, 4429-4442.	5.3	58
10	Fundamental Insights into Proton-Coupled Electron Transfer in Soybean Lipoxygenase from Quantum Mechanical/Molecular Mechanical Free Energy Simulations. Journal of the American Chemical Society, 2018, 140, 3068-3076.	13.7	46
11	Extended Zinc AMBER Force Field (EZAFF). Journal of Chemical Theory and Computation, 2018, 14, 242-254.	5.3	37
12	Formation of an unusual glutamine tautomer in a blue light using flavin photocycle characterizes the light-adapted state. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 26626-26632.	7.1	34
13	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
14	Parametrization of Trivalent and Tetravalent Metal Ions for the OPC3, OPC, TIP3P-FB, and TIP4P-FB Water Models. Journal of Chemical Theory and Computation, 2021, 17, 2342-2354.	5.3	23
15	Using Ligand-Induced Protein Chemical Shift Perturbations To Determine Proteinâ€“Ligand Structures. Biochemistry, 2017, 56, 2349-2362.	2.5	21
16	Conformational Motions and Water Networks at the Î±/Î² Interface inE. coliRibonucleotide Reductase. Journal of the American Chemical Society, 2020, 142, 13768-13778.	13.7	21
17	Environmental Effects on Guanine-Thymine Mispair Tautomerization Explored with Quantum Mechanical/Molecular Mechanical Free Energy Simulations. Journal of the American Chemical Society, 2020, 142, 11183-11191.	13.7	20
18	KECSA-Movable Type Implicit Solvation Model (KMTISM). Journal of Chemical Theory and Computation, 2015, 11, 667-682.	5.3	19

#	Article	IF	Citations
19	Impact of Mutations on the Binding Pocket of Soybean Lipoxygenase: Implications for Proton-Coupled Electron Transfer. Journal of Physical Chemistry Letters, 2018, 9, 6444-6449.	4.6	10
20	Metal Ion Capture Mechanism of a Copper Metallochaperone. Biochemistry, 2016, 55, 501-509.	2.5	9
21	Substrate-to-Product Conversion Facilitates Active Site Loop Opening in Yeast Enolase: A Molecular Dynamics Study. ACS Catalysis, 2019, 9, 8985-8990.	11.2	9
22	EFFECTS OF STRUCTURAL MODIFICATION ON THE GROUND STATE OF METALLABENZENES: SINGLET VERSUS TRIPLET STATE. Journal of Theoretical and Computational Chemistry, 2011, 10, 861-874.	1.8	5
23	Theoretical Study of Shallow Distance Dependence of Proton-Coupled Electron Transfer in Oligoproline Peptides. Journal of the American Chemical Society, 2020, 142, 13795-13804.	13.7	5
24	Bridging the 12-6-4 Model and the Fluctuating Charge Model. Frontiers in Chemistry, 2021, 9, 721960.	3.6	4
25	Parameterization of a Dioxygen Binding Metal Site Using the MCPB.py Program. Methods in Molecular Biology, 2021, 2199, 257-275.	0.9	3
26	Investigation of the pKa of the Nucleophilic O2â€² of the Hairpin Ribozyme. Journal of Physical Chemistry B, 2021, 125, 11869-11883.	2.6	2