Pengfei Li

List of Publications by Year in Descending Order

26 papers	1,640 citations	15 h-index	28 g-index
28 ext. papers	2,200 ext. citations	9.7 avg, IF	5.56 L-index

#	Paper	IF	Citations
26	Parameterization of a Dioxygen Binding Metal Site Using the MCPB.py Program. *Methods in Molecular Biology*, **2021**, 2199, 257-275	1.4	
25	Investigation of the p of the Nucleophilic O2Sof the Hairpin Ribozyme. *Journal of Physical Chemistry B*, **2021**, 125, 11869-11883	3.4	1
24	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	6.4	10
23	Bridging the 12-6-4 Model and the Fluctuating Charge Model. *Frontiers in Chemistry*, **2021**, 9, 721960	5	1
22	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	6.1	19
21	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	16.4	10
20	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	6.4	18
19	Conformational Motions and Water Networks at the /I Interface in Ribonucleotide Reductase. *Journal of the American Chemical Society*, **2020**, 142, 13768-13778	16.4	11
18	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	11.5	17
17	Theoretical Study of Shallow Distance Dependence of Proton-Coupled Electron Transfer in Oligoproline Peptides. *Journal of the American Chemical Society*, **2020**, 142, 13795-13804	16.4	1
16	Substrate-to-Product Conversion Facilitates Active Site Loop Opening in Yeast Enolase: A Molecular Dynamics Study. *ACS Catalysis*, **2019**, 9, 8985-8990	13.1	5
15	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	16.4	30
14	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	13.1	87
13	Extended Zinc AMBER Force Field (EZAFF). *Journal of Chemical Theory and Computation*, **2018**, 14, 242-254	5.4	20
12	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	6.4	7
11	Using Ligand-Induced Protein Chemical Shift Perturbations To Determine Protein-Ligand Structures. *Biochemistry*, **2017**, 56, 2349-2362	3.2	18
10	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	3.5	21

List of Publications

9	Metal Ion Modeling Using Classical Mechanics. *Chemical Reviews*, **2017**, 117, 1564-1686	68.1	189
8	MCPB.py: A Python Based Metal Center Parameter Builder. *Journal of Chemical Information and Modeling*, **2016**, 56, 599-604	6.1	237
7	Metal Ion Capture Mechanism of a Copper Metallochaperone. *Biochemistry*, **2016**, 55, 501-9	3.2	6
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, 883-95	3.4	150
5	KECSA-Movable Type Implicit Solvation Model (KMTISM). *Journal of Chemical Theory and Computation*, **2015**, 11, 667-82	6.4	16
4	Systematic Parameterization of Monovalent Ions Employing the Nonbonded Model. *Journal of Chemical Theory and Computation*, **2015**, 11, 1645-57	6.4	195
3	Taking into Account the Ion-induced Dipole Interaction in the Nonbonded Model of Ions. *Journal of Chemical Theory and Computation*, **2014**, 10, 289-297	6.4	201
2	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	6.4	365
1	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