Ray Luo

List of Publications by Year in descending order

131 papers	17,605 citations	61857 43 h-index	13727 129 g-index
135 all docs	135 docs citations	135 times ranked	18330 citing authors

#	Article	IF	Citations
1	The Amber biomolecular simulation programs. Journal of Computational Chemistry, 2005, 26, 1668-1688.	1.5	7,742
2	A point-charge force field for molecular mechanics simulations of proteins based on condensed-phase quantum mechanical calculations. Journal of Computational Chemistry, 2003, 24, 1999-2012.	1.5	4,028
3	Accelerated Poisson-Boltzmann calculations for static and dynamic systems. Journal of Computational Chemistry, 2002, 23, 1244-1253.	1.5	421
4	Recent Developments and Applications of the MMPBSA Method. Frontiers in Molecular Biosciences, 2017, 4, 87.	1.6	374
5	Implicit Nonpolar Solvent Models. Journal of Physical Chemistry B, 2007, 111, 12263-12274.	1.2	206
6	New-Generation Amber United-Atom Force Field. Journal of Physical Chemistry B, 2006, 110, 13166-13176.	1.2	176
7	Virtual screening using molecular simulations. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1940-1951.	1.5	171
8	Calculating proteinâ€“ligand binding affinities with MMPBSA: Method and error analysis. Journal of Computational Chemistry, 2016, 37, 2436-2446.	1.5	169
9	The IDP-Specific Force Field ff14IDPSFF Improves the Conformer Sampling of Intrinsically Disordered Proteins. Journal of Chemical Information and Modeling, 2017, 57, 1166-1178.	2.5	157
10	A Poissonâ€“Boltzmann dynamics method with nonperiodic boundary condition. Journal of Chemical Physics, 2003, 119, 11035-11047.	1.2	155
11	How Well Does Poissonâ^'Boltzmann Implicit Solvent Agree with Explicit Solvent? A Quantitative Analysis. Journal of Physical Chemistry B, 2006, 110, 18680-18687.	1.2	153
12	Development of Polarizable Models for Molecular Mechanical Calculations I: Parameterization of Atomic Polarizability. Journal of Physical Chemistry B, 2011, 115, 3091-3099.	1.2	137
13	An Analysis of the Interactions between the Semâ^'5 SH3 Domain and Its Ligands Using Molecular Dynamics, Free Energy Calculations, and Sequence Analysis. Journal of the American Chemical Society, 2001, 123, 3986-3994.	6.6	130
14	Development of Polarizable Models for Molecular Mechanical Calculations II: Induced Dipole Models Significantly Improve Accuracy of Intermolecular Interaction Energies. Journal of Physical Chemistry B, 2011, 115, 3100-3111.	1.2	116
15	New Force Field on Modeling Intrinsically Disordered Proteins. Chemical Biology and Drug Design, 2014, 84, 253-269.	1.5	110
16	Binding Induced Folding in p53â^'MDM2 Complex. Journal of the American Chemical Society, 2007, 129, 2930-2937.	6.6	107
17	Comparison of generalized born and poisson models: Energetics and dynamics of HIV protease. Journal of Computational Chemistry, 2000, 21, 295-309.	1.5	98
18	Performance of Nonlinear Finite-Difference Poissonâ^'Boltzmann Solvers. Journal of Chemical Theory and Computation, 2010, 6, 203-211.	2.3	89

#	Article	IF	Citations
19	The Physical Basis of Nucleic Acid Base Stacking in Water. Biophysical Journal, 2001, 80, 140-148.	0.2	87
20	Regulation of the Hippo Pathway by Phosphatidic Acid-Mediated Lipid-Protein Interaction. Molecular Cell, 2018, 72, 328-340.e8.	4.5	74
21	Assessment of linear finiteâ€difference Poissonâ€“Boltzmann solvers. Journal of Computational Chemistry, 2010, 31, 1689-1698.	1.5	73
22	Strength of Solvent-Exposed Salt-Bridges. Journal of Physical Chemistry B, 1999, 103, 727-736.	1.2	71
23	Test and Evaluation of ff99IDPs Force Field for Intrinsically Disordered Proteins. Journal of Chemical Information and Modeling, 2015, 55, 1021-1029.	2.5	68
24	ff14IDPs force field improving the conformation sampling of intrinsically disordered proteins. Chemical Biology and Drug Design, 2017, 89, 5-15.	1.5	67
25	Recent Force Field Strategies for Intrinsically Disordered Proteins. Journal of Chemical Information and Modeling, 2021, 61, 1037-1047.	2.5	67
26	Force field influences in Î²-hairpin folding simulations. Protein Science, 2006, 15, 2642-2655.	3.1	63
27	Intrinsically disordered proteinâ€specific force field <scp>CHARMM</scp>36<scp>IDPSFF</scp>. Chemical Biology and Drug Design, 2018, 92, 1722-1735.	1.5	62
28	Molecular Dynamics Simulations of p53 DNA-Binding Domain. Journal of Physical Chemistry B, 2007, 111, 11538-11545.	1.2	60
29	Development of Polarizable Models for Molecular Mechanical Calculations. 4. van der Waals Parametrization. Journal of Physical Chemistry B, 2012, 116, 7088-7101.	1.2	60
30	Reducing Grid Dependence in Finite-Difference Poissonâ€“Boltzmann Calculations. Journal of Chemical Theory and Computation, 2012, 8, 2741-2751.	2.3	58
31	Inhibition Kinetics and Emodin Cocrystal Structure of a Type II Polyketide Ketoreductase[,]. Biochemistry, 2008, 47, 1837-1847.	1.2	57
32	Comprehensive Structural and Biochemical Analysis of the Terminal Myxalamid Reductase Domain for the Engineered Production of Primary Alcohols. Chemistry and Biology, 2015, 22, 1018-1029.	6.2	56
33	Recent Developments in Free Energy Calculations for Drug Discovery. Frontiers in Molecular Biosciences, 2021, 8, 712085.	1.6	56
34	pKaShifts in Small Molecules and HIV Protease:Â Electrostatics and Conformation. Journal of the American Chemical Society, 1998, 120, 6138-6146.	6.6	55
35	Environment-Specific Force Field for Intrinsically Disordered and Ordered Proteins. Journal of Chemical Information and Modeling, 2020, 60, 2257-2267.	2.5	55
36	Ligand-receptor docking with the Mining Minima optimizer. Journal of Computer-Aided Molecular Design, 2001, 15, 157-171.	1.3	51

#	Article	IF	Citations
37	Achieving energy conservation in Poissonâ€“Boltzmann molecular dynamics: Accuracy and precision with finite-difference algorithms. Chemical Physics Letters, 2009, 468, 112-118.	1.2	50
38	Synthetic Adenine Receptors:Â Direct Calculation of Binding Affinity and Entropy. Journal of the American Chemical Society, 2000, 122, 2934-2937.	6.6	49
39	Overcoming entropic barrier with coupled sampling at dual resolutions. Journal of Chemical Physics, 2005, 123, 194904.	1.2	49
40	Development of Polarizable Models for Molecular Mechanical Calculations. 3. Polarizable Water Models Conforming to Thole Polarization Screening Schemes. Journal of Physical Chemistry B, 2012, 116, 7999-8008.	1.2	49
41	On removal of charge singularity in Poissonâ€“Boltzmann equation. Journal of Chemical Physics, 2009, 130, 145101.	1.2	47
42	Enhanced ab initio protein folding simulations in Poissonâ€“Boltzmann molecular dynamics with self-guiding forces. Journal of Molecular Graphics and Modelling, 2004, 22, 415-424.	1.3	46
43	Physical scoring function based on AMBER force field and Poisson-Boltzmann implicit solvent for protein structure prediction. Proteins: Structure, Function and Bioinformatics, 2004, 56, 475-486.	1.5	46
44	Is Poisson-Boltzmann theory insufficient for protein folding simulations?. Journal of Chemical Physics, 2006, 124, 034902.	1.2	44
45	Quantitative analysis of Poissonâ€“Boltzmann implicit solvent in molecular dynamics. Physical Chemistry Chemical Physics, 2010, 12, 1194-1202.	1.3	43
46	Well-Balanced Force Field ff03CMAP for Folded and Disordered Proteins. Journal of Chemical Theory and Computation, 2019, 15, 6769-6780.	2.3	43
47	Molecular basis for interactions between an acyl carrier protein and a ketosynthase. Nature Chemical Biology, 2019, 15, 669-671.	3.9	41
48	Interpreting trends in the binding of cyclic ureas to HIV-1 protease. Journal of Molecular Biology, 2001, 309, 507-517.	2.0	39
49	Dielectric Screening Treatment of Electrostatic Solvation. Journal of Physical Chemistry B, 1997, 101, 11226-11236.	1.2	37
50	Extensive tests and evaluation of the CHARMM36IDPSFF force field for intrinsically disordered proteins and folded proteins. Physical Chemistry Chemical Physics, 2019, 21, 21918-21931.	1.3	37
51	Nucleic acid base-pairing and N-methylacetamide self-association in chloroform: affinity and conformation. Biophysical Chemistry, 1999, 78, 183-193.	1.5	36
52	Conformational Selection and Induced Fit in Specific Antibody and Antigen Recognition: SPE7 as a Case Study. Journal of Physical Chemistry B, 2013, 117, 4912-4923.	1.2	36
53	Exploring accurate Poissonâ€“Boltzmann methods for biomolecular simulations. Computational and Theoretical Chemistry, 2013, 1024, 34-44.	1.1	35
54	Synergistic Allosteric Mechanism of Fructose-1,6-bisphosphate and Serine for Pyruvate Kinase M2 via Dynamics Fluctuation Network Analysis. Journal of Chemical Information and Modeling, 2016, 56, 1184-1192.	2.5	33

#	Article	IF	Citations
55	Development of a High-Throughput, In Vivo Selection Platform for NADPH-Dependent Reactions Based on Redox Balance Principles. ACS Synthetic Biology, 2018, 7, 1715-1721.	1.9	33
56	Dielectric boundary force in numerical Poissonâ€“Boltzmann methods: Theory and numerical strategies. Chemical Physics Letters, 2011, 514, 368-373.	1.2	30
57	All-Atom Computer Simulations of Amyloid Fibrils Disaggregation. Biophysical Journal, 2008, 95, 5037-5047.	0.2	29
58	Functional Census of Mutation Sequence Spaces: The Example of p53 Cancer Rescue Mutants. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2006, 3, 114-125.	1.9	28
59	A Revised Density Function for Molecular Surface Calculation in Continuum Solvent Models. Journal of Chemical Theory and Computation, 2010, 6, 1157-1169.	2.3	28
60	Electrostatic forces in the Poisson-Boltzmann systems. Journal of Chemical Physics, 2013, 139, 094106.	1.2	27
61	Applications of MMPBSA to Membrane Proteins I: Efficient Numerical Solutions of Periodic Poissonâ€“Boltzmann Equation. Journal of Chemical Information and Modeling, 2015, 55, 2187-2199.	2.5	27
62	Heterogeneous Dielectric Implicit Membrane Model for the Calculation of MMPBSA Binding Free Energies. Journal of Chemical Information and Modeling, 2019, 59, 3041-3056.	2.5	27
63	Continuum Polarizable Force Field within the Poissonâˆ’Boltzmann Framework. Journal of Physical Chemistry B, 2008, 112, 7675-7688.	1.2	26
64	Roles of Boundary Conditions in DNA Simulations: Analysis of Ion Distributions with the Finite-Difference Poisson-Boltzmann Method. Biophysical Journal, 2009, 97, 554-562.	0.2	26
65	Dielectric pressure in continuum electrostatic solvation of biomolecules. Physical Chemistry Chemical Physics, 2012, 14, 15917.	1.3	26
66	Numerical Poissonâ€“Boltzmann model for continuum membrane systems. Chemical Physics Letters, 2013, 555, 274-281.	1.2	26
67	Development of Polarizable Gaussian Model for Molecular Mechanical Calculations I: Atomic Polarizability Parameterization To Reproduce ab Initio Anisotropy. Journal of Chemical Theory and Computation, 2019, 15, 1146-1158.	2.3	26
68	Confronting the problem of interconnected structural changes in the comparative modeling of proteins. Proteins: Structure, Function and Bioinformatics, 1995, 23, 327-336.	1.5	25
69	Recent progress in adapting Poissonâ€“Boltzmann methods to molecular simulations. Journal of Theoretical and Computational Chemistry, 2014, 13, 1430001.	1.8	25
70	Structural Insights into Anthranilate Priming during Type II Polyketide Biosynthesis. ACS Chemical Biology, 2016, 11, 95-103.	1.6	25
71	On-the-Fly Numerical Surface Integration for Finite-Difference Poissonâ€“Boltzmann Methods. Journal of Chemical Theory and Computation, 2011, 7, 3608-3619.	2.3	24
72	Dynamics Correlation Network for Allosteric Switching of PreQ1 Riboswitch. Scientific Reports, 2016, 6, 31005.	1.6	24

#	Article	IF	Citations
73	Modeling Membrane Proteinâ€“Ligand Binding Interactions: The Human Purinergic Platelet Receptor. Journal of Physical Chemistry B, 2016, 120, 12293-12304.	1.2	24
74	Computational Studies of Intrinsically Disordered Proteins. Journal of Physical Chemistry B, 2018, 122, 10455-10469.	1.2	24
75	Elucidation of <scp>WW</scp> domain ligand binding specificities in the Hippo pathway reveals <scp>STXBP</scp> 4 as <scp>YAP</scp> inhibitor. EMBO Journal, 2020, 39, e102406.	3.5	23
76	The Hippo pathway kinases LATS1 and LATS2 attenuate cellular responses to heavy metals through phosphorylating MTF1. Nature Cell Biology, 2022, 24, 74-87.	4.6	22
77	An Oxetane-Based Polyketide Surrogate To Probe Substrate Binding in a Polyketide Synthase. Journal of the American Chemical Society, 2018, 140, 4961-4964.	6.6	21
78	Interplay of secondary structures and side-chain contacts in the denatured state of BBA1. Journal of Chemical Physics, 2004, 121, 2412-2421.	1.2	20
79	Continuum treatment of electronic polarization effect. Journal of Chemical Physics, 2007, 126, 094103.	1.2	20
80	Protein Stability Prediction:â€‰ A Poissonâ€“Boltzmann Approach. Journal of Physical Chemistry B, 2008, 112, 1875-1883.	1.2	20
81	Computational Study of KNI-272, a Potent Inhibitor of HIV-1 Protease: On the Mechanism of Preorganization. Journal of Physical Chemistry B, 1999, 103, 1031-1044.	1.2	19
82	A Continuum Poissonâ€“Boltzmann Model for Membrane Channel Proteins. Journal of Chemical Theory and Computation, 2017, 13, 3398-3412.	2.3	19
83	Efficient formulation of polarizable Gaussian multipole electrostatics for biomolecular simulations. Journal of Chemical Physics, 2020, 153, 114116.	1.2	19
84	Structural and functional implications of p53 missense cancer mutations. PMC Biophysics, 2009, 2, 5.	2.2	17
85	Exploring a charge-central strategy in the solution of Poisson's equation for biomolecular applications. Physical Chemistry Chemical Physics, 2013, 15, 129-141.	1.3	17
86	Conformation dynamics of the intrinsically disordered protein c-Myb with the ff99IDPs force field. RSC Advances, 2017, 7, 29713-29721.	1.7	17
87	Biological applications of classical electrostatics methods. Journal of Theoretical and Computational Chemistry, 2014, 13, 1440008.	1.8	16
88	Synergistic Modification Induced Specific Recognition between Histone and TRIM24 via Fluctuation Correlation Network Analysis. Scientific Reports, 2016, 6, 24587.	1.6	15
89	Exploring a coarse-grained distributive strategy for finite-difference Poissonâ€“Boltzmann calculations. Journal of Molecular Modeling, 2011, 17, 1985-1996.	0.8	13
90	Kink turn sRNA folding upon L7Ae binding using molecular dynamics simulations. Physical Chemistry Chemical Physics, 2013, 15, 18510.	1.3	13

#	Article	IF	Citations
91	Acceleration of Linear Finite-Difference Poissonâ€“Boltzmann Methods on Graphics Processing Units. Journal of Chemical Theory and Computation, 2017, 13, 3378-3387.	2.3	13
92	Atomistic Mechanism of MicroRNA Translation Upregulation via Molecular Dynamics Simulations. PLoS ONE, 2012, 7, e43788.	1.1	13
93	Poissonâ€“Boltzmann Implicit Solvation Models. Annual Reports in Computational Chemistry, 2012, , 149-162.	0.9	12
94	Recognition Mechanism between Lac Repressor and DNA with Correlation Network Analysis. Journal of Physical Chemistry B, 2015, 119, 2844-2856.	1.2	12
95	Allosteric Autoinhibition Pathway in Transcription Factor ERG: Dynamics Network and Mutant Experimental Evaluations. Journal of Chemical Information and Modeling, 2017, 57, 1153-1165.	2.5	12
96	Dynamical important residue network (DIRN): network inference via conformational change. Bioinformatics, 2019, 35, 4664-4670.	1.8	12
97	Molecular Basis for Polyketide Ketoreductaseâ€“Substrate Interactions. International Journal of Molecular Sciences, 2020, 21, 7562.	1.8	12
98	PyRESP: A Program for Electrostatic Parameterizations of Additive and Induced Dipole Polarizable Force Fields. Journal of Chemical Theory and Computation, 2022, 18, 3654-3670.	2.3	12
99	A multi-scale method for dynamics simulation in continuum solvent models. I: Finite-difference algorithm for Navierâ€“Stokes equation. Chemical Physics Letters, 2014, 616-617, 67-74.	1.2	11
100	Computational structural enzymology methodologies for the study and engineering of fatty acid synthases, polyketide synthases and nonribosomal peptide synthetases. Methods in Enzymology, 2019, 622, 375-409.	0.4	11
101	A 2,3-dialkoxynaphthalene-based naphthocage. Chemical Communications, 2020, 56, 888-891.	2.2	11
102	Development of a Pantetheine Force Field Library for Molecular Modeling. Journal of Chemical Information and Modeling, 2021, 61, 856-868.	2.5	11
103	Estimating the Roles of Protonation and Electronic Polarization in Absolute Binding Affinity Simulations. Journal of Chemical Theory and Computation, 2021, 17, 2541-2555.	2.3	11
104	Molecular mechanisms of functional rescue mediated by P53 tumor suppressor mutations. Biophysical Chemistry, 2009, 145, 37-44.	1.5	10
105	A semi-implicit augmented IIM for Navierâ€“Stokes equations with open, traction, or free boundary conditions. Journal of Computational Physics, 2015, 297, 182-193.	1.9	10
106	Numerical interpretation of molecular surface field in dielectric modeling of solvation. Journal of Computational Chemistry, 2017, 38, 1057-1070.	1.5	10
107	Improved Poissonâ€“Boltzmann Methods for High-Performance Computing. Journal of Chemical Theory and Computation, 2019, 15, 6190-6202.	2.3	10
108	Leveraging Oxidative Stress to Regulate Redox Balance-Based, In Vivo Growth Selections for Oxygenase Engineering. ACS Synthetic Biology, 2020, 9, 3124-3133.	1.9	10

#	Article	IF	Citations
109	Growth-Based, High-Throughput Selection for NADH Preference in an Oxygen-Dependent Biocatalyst. ACS Synthetic Biology, 2021, 10, 2359-2370.	1.9	10
110	Stress tensor and constant pressure simulation for polarizable Gaussian multipole model. Journal of Chemical Physics, 2022, 156, 114114.	1.2	10
111	Ionic Solution: What Goes Right and Wrong with Continuum Solvation Modeling. Journal of Physical Chemistry B, 2017, 121, 11169-11179.	1.2	9
112	Robustness and Efficiency of Poissonâ€“Boltzmann Modeling on Graphics Processing Units. Journal of Chemical Information and Modeling, 2019, 59, 409-420.	2.5	9
113	Impact of low-frequency hotspot mutation R282Q on the structure of p53 DNA-binding domain as revealed by crystallography at 1.54â€…Ã… resolution. Acta Crystallographica Section D: Biological Crystallography, 2008, 64, 471-477.	2.5	8
114	Balancing Simulation Accuracy and Efficiency with the Amber United Atom Force Field. Journal of Physical Chemistry B, 2010, 114, 2886-2893.	1.2	8
115	Charge Central Interpretation of the Full Nonlinear PB Equation: Implications for Accurate and Scalable Modeling of Solvation Interactions. Journal of Physical Chemistry B, 2016, 120, 8707-8721.	1.2	8
116	Computational Analysis for the Rational Design of Anti-Amyloid Beta (AÎ²) Antibodies. Journal of Physical Chemistry B, 2018, 122, 4521-4536.	1.2	8
117	Motif-dependent immune co-receptor interactome profiling by photoaffinity chemical proteomics. Cell Chemical Biology, 2022, 29, 1024-1036.e5.	2.5	8
118	Specific Recognition Mechanism between RNA and the KH3 Domain of Nova-2 Protein. Journal of Physical Chemistry B, 2014, 118, 12426-12434.	1.2	7
119	An efficient secondâ€order poissonâ€“boltzmann method. Journal of Computational Chemistry, 2019, 40, 1257-1269.	1.5	7
120	Heparin-Assisted Amyloidogenesis Uncovered through Molecular Dynamics Simulations. ACS Omega, 2022, 7, 15132-15144.	1.6	7
121	Allosteric pathways in tetrahydrofolate sensing riboswitch with dynamics correlation network. Molecular BioSystems, 2017, 13, 156-164.	2.9	6
122	Modeling Molecular Recognition: Theory and Application. Journal of Biomolecular Structure and Dynamics, 2000, 17, 89-94.	2.0	5
123	Crystal Structure of StnA for the Biosynthesis of Antitumor Drug Streptonigrin Reveals a Unique Substrate Binding Mode. Scientific Reports, 2017, 7, 40254.	1.6	5
124	Order-disorder transition of intrinsically disordered kinase inducible transactivation domain of CREB. Journal of Chemical Physics, 2018, 148, 225101.	1.2	5
125	Engineering Embdenâ€“Meyerhofâ€“Parnas Glycolysis to Generate Noncanonical Reducing Power. ACS Catalysis, 2022, 12, 8582-8592.	5.5	5
126	Widespread but Small-Scale Changes in the Structural and Dynamic Properties of Vaccinia Virus Poly(A) Polymerase upon Association with Its Processivity Factor in Solution. Biochemistry, 2010, 49, 6247-6262.	1.2	4

#	Article	IF	Citations
127	Machine-Learned Molecular Surface and Its Application to Implicit Solvent Simulations. Journal of Chemical Theory and Computation, 2021, 17, 6214-6224.	2.3	4
128	Exploring a multi-scale method for molecular simulation in continuum solvent model: Explicit simulation of continuum solvent as an incompressible fluid. Journal of Chemical Physics, 2017, 147, 214112.	1.2	3
129	In Vivo, High-Throughput Selection of Thermostable Cyclohexanone Monooxygenase (CHMO). Catalysts, 2020, 10, 935.	1.6	2
130	Engineering a Coenzyme A Detour To Expand the Product Scope and Enhance the Selectivity of the Ehrlich Pathway. ACS Synthetic Biology, 2018, 7, 2758-2764.	1.9	1
131	Improved Accuracy and Convergence of Intrinsically Disordered Protein Molecular Dynamics Simulations Using the ff14IDPSFF Force Field. Biophysical Journal, 2018, 114, 432a.	0.2	1