Ray Luo

List of Publications by Citations

126 papers	14,303 citations	39 h-index	119 g-index
135 ext. papers	16,097 ext. citations	4.9 avg, IF	6.12 L-index

#	Paper	IF	Citations
126	The Amber biomolecular simulation programs. *Journal of Computational Chemistry*, **2005**, 26, 1668-88	3.5	6155
125	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	3.5	3573
124	Accelerated Poisson-Boltzmann calculations for static and dynamic systems. *Journal of Computational Chemistry*, **2002**, 23, 1244-53	3.5	368
123	Recent Developments and Applications of the MMPBSA Method. *Frontiers in Molecular Biosciences*, **2017**, 4, 87	5.6	229
122	Implicit nonpolar solvent models. *Journal of Physical Chemistry B*, **2007**, 111, 12263-74	3.4	167
121	New-generation amber united-atom force field. *Journal of Physical Chemistry B*, **2006**, 110, 13166-76	3.4	157
120	A Poisson–Boltzmann dynamics method with nonperiodic boundary condition. *Journal of Chemical Physics*, **2003**, 119, 11035-11047	3.9	145
119	How well does Poisson-Boltzmann implicit solvent agree with explicit solvent? A quantitative analysis. *Journal of Physical Chemistry B*, **2006**, 110, 18680-7	3.4	135
118	Virtual screening using molecular simulations. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 1940-51	4.2	128
117	An analysis of the interactions between the Sem-5 SH3 domain and its ligands using molecular dynamics, free energy calculations, and sequence analysis. *Journal of the American Chemical Society*, **2001**, 123, 3986-94	16.4	121
116	Development of polarizable models for molecular mechanical calculations I: parameterization of atomic polarizability. *Journal of Physical Chemistry B*, **2011**, 115, 3091-9	3.4	114
115	The IDP-Specific Force Field ff14IDPSFF Improves the Conformer Sampling of Intrinsically Disordered Proteins. *Journal of Chemical Information and Modeling*, **2017**, 57, 1166-1178	6.1	108
114	Calculating protein-ligand binding affinities with MMPBSA: Method and error analysis. *Journal of Computational Chemistry*, **2016**, 37, 2436-46	3.5	108
113	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, 3100-11	3.4	101
112	Binding induced folding in p53-MDM2 complex. *Journal of the American Chemical Society*, **2007**, 129, 2930-7	16.4	98
111	Comparison of generalized born and poisson models: Energetics and dynamics of HIV protease. *Journal of Computational Chemistry*, **2000**, 21, 295-309	3.5	93
110	New force field on modeling intrinsically disordered proteins. *Chemical Biology and Drug Design*, **2014**, 84, 253-69	2.9	84

109	The physical basis of nucleic acid base stacking in water. *Biophysical Journal*, **2001**, 80, 140-8	2.9	84
108	Performance of Nonlinear Finite-Difference Poisson-Boltzmann Solvers. *Journal of Chemical Theory and Computation*, **2010**, 6, 203-211	6.4	72
107	Strength of Solvent-Exposed Salt-Bridges. *Journal of Physical Chemistry B*, **1999**, 103, 727-736	3.4	67
106	Force field influences in beta-hairpin folding simulations. *Protein Science*, **2006**, 15, 2642-55	6.3	60
105	Assessment of linear finite-difference Poisson-Boltzmann solvers. *Journal of Computational Chemistry*, **2010**, 31, 1689-98	3.5	58
104	Test and Evaluation of ff99IDPs Force Field for Intrinsically Disordered Proteins. *Journal of Chemical Information and Modeling*, **2015**, 55, 1021-9	6.1	53
103	Inhibition kinetics and emodin cocrystal structure of a type II polyketide ketoreductase. *Biochemistry*, **2008**, 47, 1837-47	3.2	53
102	pKaShifts in Small Molecules and HIV Protease:Electrostatics and Conformation. *Journal of the American Chemical Society*, **1998**, 120, 6138-6146	16.4	52
101	Molecular dynamics simulations of p53 DNA-binding domain. *Journal of Physical Chemistry B*, **2007**, 111, 11538-45	3.4	48
100	Ligand-receptor docking with the Mining Minima optimizer. *Journal of Computer-Aided Molecular Design*, **2001**, 15, 157-71	4.2	48
99	Synthetic Adenine Receptors:Direct Calculation of Binding Affinity and Entropy. *Journal of the American Chemical Society*, **2000**, 122, 2934-2937	16.4	48
98	Reducing grid-dependence in finite-difference Poisson-Boltzmann calculations. *Journal of Chemical Theory and Computation*, **2012**, 8, 2741-2751	6.4	46
97	Development of polarizable models for molecular mechanical calculations. 4. van der Waals parametrization. *Journal of Physical Chemistry B*, **2012**, 116, 7088-101	3.4	44
96	Overcoming entropic barrier with coupled sampling at dual resolutions. *Journal of Chemical Physics*, **2005**, 123, 194904	3.9	44
95	Comprehensive Structural and Biochemical Analysis of the Terminal Myxalamid Reductase Domain for the Engineered Production of Primary Alcohols. *Chemistry and Biology*, **2015**, 22, 1018-29		43
94	On removal of charge singularity in Poisson-Boltzmann equation. *Journal of Chemical Physics*, **2009**, 130, 145101	3.9	43
93	Physical scoring function based on AMBER force field and Poisson-Boltzmann implicit solvent for protein structure prediction. *Proteins: Structure, Function and Bioinformatics*, **2004**, 56, 475-86	4.2	43
92	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	3.4	42

91	Achieving Energy Conservation in Poisson-Boltzmann Molecular Dynamics: Accuracy and Precision with Finite-Difference Algorithms. *Chemical Physics Letters*, **2009**, 468, 112-118	2.5	41
90	Regulation of the Hippo Pathway by Phosphatidic Acid-Mediated Lipid-Protein Interaction. *Molecular Cell*, **2018**, 72, 328-340.e8	17.6	41
89	Is Poisson-Boltzmann theory insufficient for protein folding simulations?. *Journal of Chemical Physics*, **2006**, 124, 034902	3.9	40
88	Enhanced ab initio protein folding simulations in Poisson-Boltzmann molecular dynamics with self-guiding forces. *Journal of Molecular Graphics and Modelling*, **2004**, 22, 415-24	2.8	39
87	Interpreting trends in the binding of cyclic ureas to HIV-1 protease. *Journal of Molecular Biology*, **2001**, 309, 507-17	6.5	37
86	Intrinsically disordered protein-specific force field CHARMM36IDPSFF. *Chemical Biology and Drug Design*, **2018**, 92, 1722-1735	2.9	36
85	Dielectric Screening Treatment of Electrostatic Solvation. *Journal of Physical Chemistry B*, **1997**, 101, 11226-11236	3.4	35
84	Nucleic acid base-pairing and N-methylacetamide self-association in chloroform: affinity and conformation. *Biophysical Chemistry*, **1999**, 78, 183-93	3.5	35
83	Quantitative analysis of Poisson-Boltzmann implicit solvent in molecular dynamics. *Physical Chemistry Chemical Physics*, **2010**, 12, 1194-202	3.6	34
82	Environment-Specific Force Field for Intrinsically Disordered and Ordered Proteins. *Journal of Chemical Information and Modeling*, **2020**, 60, 2257-2267	6.1	32
81	Exploring accurate Poisson-Boltzmann methods for biomolecular simulations. *Computational and Theoretical Chemistry*, **2013**, 1024, 34-44	2	32
80	All-atom computer simulations of amyloid fibrils disaggregation. *Biophysical Journal*, **2008**, 95, 5037-47	2.9	29
79	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	6.1	29
78	Conformational selection and induced fit in specific antibody and antigen recognition: SPE7 as a case study. *Journal of Physical Chemistry B*, **2013**, 117, 4912-23	3.4	28
77	Well-Balanced Force Field 03 for Folded and Disordered Proteins. *Journal of Chemical Theory and Computation*, **2019**, 15, 6769-6780	6.4	27
76	Dielectric Boundary Forces in Numerical Poisson-Boltzmann Methods: Theory and Numerical Strategies. *Chemical Physics Letters*, **2011**, 514, 368-373	2.5	27
75	Extensive tests and evaluation of the CHARMM36IDPSFF force field for intrinsically disordered proteins and folded proteins. *Physical Chemistry Chemical Physics*, **2019**, 21, 21918-21931	3.6	25
74	Molecular basis for interactions between an acyl carrier protein and a ketosynthase. *Nature Chemical Biology*, **2019**, 15, 669-671	11.7	25

73	Electrostatic forces in the Poisson-Boltzmann systems. *Journal of Chemical Physics*, **2013**, 139, 094106	3.9	25
72	A revised density function for molecular surface definition in continuum solvent models. *Journal of Chemical Theory and Computation*, **2010**, 6, 1157-1169	6.4	25
71	Roles of boundary conditions in DNA simulations: analysis of ion distributions with the finite-difference Poisson-Boltzmann method. *Biophysical Journal*, **2009**, 97, 554-62	2.9	25
70	Recent progress in adapting Poisson-Boltzmann methods to molecular simulations. *Journal of Theoretical and Computational Chemistry*, **2014**, 13, 1430001	1.8	24
69	Recent Force Field Strategies for Intrinsically Disordered Proteins. *Journal of Chemical Information and Modeling*, **2021**, 61, 1037-1047	6.1	24
68	Applications of MMPBSA to Membrane Proteins I: Efficient Numerical Solutions of Periodic Poisson-Boltzmann Equation. *Journal of Chemical Information and Modeling*, **2015**, 55, 2187-99	6.1	23
67	Numerical Poisson-Boltzmann Model for Continuum Membrane Systems. *Chemical Physics Letters*, **2013**, 555, 274-281	2.5	23
66	Dielectric pressure in continuum electrostatic solvation of biomolecules. *Physical Chemistry Chemical Physics*, **2012**, 14, 15917-25	3.6	23
65	Functional census of mutation sequence spaces: the example of p53 cancer rescue mutants. *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, **2006**, 3, 114-25	3	22
64	On-the-fly Numerical Surface Integration for Finite-Difference Poisson-Boltzmann Methods. *Journal of Chemical Theory and Computation*, **2011**, 7, 3608-3619	6.4	21
63	Continuum polarizable force field within the Poisson-Boltzmann framework. *Journal of Physical Chemistry B*, **2008**, 112, 7675-88	3.4	20
62	Confronting the problem of interconnected structural changes in the comparative modeling of proteins. *Proteins: Structure, Function and Bioinformatics*, **1995**, 23, 327-36	4.2	20
61	Dynamics Correlation Network for Allosteric Switching of PreQ1 Riboswitch. *Scientific Reports*, **2016**, 6, 31005	4.9	20
60	Interplay of secondary structures and side-chain contacts in the denatured state of BBA1. *Journal of Chemical Physics*, **2004**, 121, 2412-21	3.9	19
59	An Oxetane-Based Polyketide Surrogate To Probe Substrate Binding in a Polyketide Synthase. *Journal of the American Chemical Society*, **2018**, 140, 4961-4964	16.4	18
58	Exploring a charge-central strategy in the solution of Poisson's equation for biomolecular applications. *Physical Chemistry Chemical Physics*, **2013**, 15, 129-41	3.6	17
57	Protein stability prediction: a Poisson-Boltzmann approach. *Journal of Physical Chemistry B*, **2008**, 112, 1875-83	3.4	17
56	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	3.4	17

55	Computational Studies of Intrinsically Disordered Proteins. *Journal of Physical Chemistry B*, **2018**, 122, 10455-10469	3.4	17
54	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	5.7	17
53	Structural Insights into Anthranilate Priming during Type II Polyketide Biosynthesis. *ACS Chemical Biology*, **2016**, 11, 95-103	4.9	16
52	A Continuum Poisson-Boltzmann Model for Membrane Channel Proteins. *Journal of Chemical Theory and Computation*, **2017**, 13, 3398-3412	6.4	15
51	Synergistic Modification Induced Specific Recognition between Histone and TRIM24 via Fluctuation Correlation Network Analysis. *Scientific Reports*, **2016**, 6, 24587	4.9	15
50	Biological applications of classical electrostatics methods. *Journal of Theoretical and Computational Chemistry*, **2014**, 13, 1440008	1.8	15
49	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	6.4	15
48	Heterogeneous Dielectric Implicit Membrane Model for the Calculation of MMPBSA Binding Free Energies. *Journal of Chemical Information and Modeling*, **2019**, 59, 3041-3056	6.1	14
47	Modeling Membrane Protein-Ligand Binding Interactions: The Human Purinergic Platelet Receptor. *Journal of Physical Chemistry B*, **2016**, 120, 12293-12304	3.4	14
46	Structural and functional implications of p53 missense cancer mutations. *PMC Biophysics*, **2009**, 2, 5		14
45	Exploring a coarse-grained distributive strategy for finite-difference Poisson-Boltzmann calculations. *Journal of Molecular Modeling*, **2011**, 17, 1985-96	2	13
44	Continuum treatment of electronic polarization effect. *Journal of Chemical Physics*, **2007**, 126, 094103	3.9	13
43	Conformation Dynamics of the Intrinsically Disordered Protein c-Myb with the Force Field. *RSC Advances*, **2017**, 7, 29713-29721	3.7	12
42	Kink turn sRNA folding upon L7Ae binding using molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2013**, 15, 18510-22	3.6	12
41	Recognition mechanism between Lac repressor and DNA with correlation network analysis. *Journal of Physical Chemistry B*, **2015**, 119, 2844-56	3.4	12
40	Allosteric Autoinhibition Pathway in Transcription Factor ERG: Dynamics Network and Mutant Experimental Evaluations. *Journal of Chemical Information and Modeling*, **2017**, 57, 1153-1165	6.1	11
39	PoissonBoltzmann Implicit Solvation Models. *Annual Reports in Computational Chemistry*, **2012**, 149-162	1.8	11
38	Atomistic mechanism of microRNA translation upregulation via molecular dynamics simulations. *PLoS ONE*, **2012**, 7, e43788	3.7	11

37	A semi-implicit augmented IIM for Navier-Stokes equations with open, traction, or free boundary conditions. *Journal of Computational Physics*, **2015**, 297, 182-193	4.1	10
36	A Multi-Scale Method for Dynamics Simulation in Continuum Solvent Models I: Finite-Difference Algorithm for Navier-Stokes Equation. *Chemical Physics Letters*, **2014**, 616-617, 67-74	2.5	10
35	Acceleration of Linear Finite-Difference Poisson-Boltzmann Methods on Graphics Processing Units. *Journal of Chemical Theory and Computation*, **2017**, 13, 3378-3387	6.4	10
34	Ionic Solution: What Goes Right and Wrong with Continuum Solvation Modeling. *Journal of Physical Chemistry B*, **2017**, 121, 11169-11179	3.4	9
33	A 2,3-dialkoxynaphthalene-based naphthocage. *Chemical Communications*, **2020**, 56, 888-891	5.8	9
32	Efficient formulation of polarizable Gaussian multipole electrostatics for biomolecular simulations. *Journal of Chemical Physics*, **2020**, 153, 114116	3.9	9
31	Recent Developments in Free Energy Calculations for Drug Discovery. *Frontiers in Molecular Biosciences*, **2021**, 8, 712085	5.6	9
30	Numerical interpretation of molecular surface field in dielectric modeling of solvation. *Journal of Computational Chemistry*, **2017**, 38, 1057-1070	3.5	8
29	Dynamical important residue network (DIRN): network inference via conformational change. *Bioinformatics*, **2019**, 35, 4664-4670	7.2	8
28	Computational Analysis for the Rational Design of Anti-Amyloid Beta (A)Antibodies. *Journal of Physical Chemistry B*, **2018**, 122, 4521-4536	3.4	8
27	Balancing simulation accuracy and efficiency with the Amber united atom force field. *Journal of Physical Chemistry B*, **2010**, 114, 2886-93	3.4	8
26	Robustness and Efficiency of Poisson-Boltzmann Modeling on Graphics Processing Units. *Journal of Chemical Information and Modeling*, **2019**, 59, 409-420	6.1	8
25	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, 8707-21	3.4	7
24	Molecular mechanisms of functional rescue mediated by P53 tumor suppressor mutations. *Biophysical Chemistry*, **2009**, 145, 37-44	3.5	7
23	Impact of low-frequency hotspot mutation R282Q on the structure of p53 DNA-binding domain as revealed by crystallography at 1.54 angstroms resolution. *Acta Crystallographica Section D: Biological Crystallography*, **2008**, 64, 471-7		7
22	Elucidation of WW domain ligand binding specificities in the Hippo pathway reveals STXBP4 as YAP inhibitor. *EMBO Journal*, **2020**, 39, e102406	13	7
21	Improved Poisson-Boltzmann Methods for High-Performance Computing. *Journal of Chemical Theory and Computation*, **2019**, 15, 6190-6202	6.4	6
20	Allosteric pathways in tetrahydrofolate sensing riboswitch with dynamics correlation network. *Molecular BioSystems*, **2016**, 13, 156-164		6

19	An efficient second-order poisson-boltzmann method. *Journal of Computational Chemistry*, **2019**, 40, 1257-1269	3.5	6
18	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	1.7	5
17	Order-disorder transition of intrinsically disordered kinase inducible transactivation domain of CREB. *Journal of Chemical Physics*, **2018**, 148, 225101	3.9	5
16	Specific recognition mechanism between RNA and the KH3 domain of Nova-2 protein. *Journal of Physical Chemistry B*, **2014**, 118, 12426-34	3.4	5
15	Crystal Structure of StnA for the Biosynthesis of Antitumor Drug Streptonigrin Reveals a Unique Substrate Binding Mode. *Scientific Reports*, **2017**, 7, 40254	4.9	4
14	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	3.9	3
13	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, 6247-62	3.2	3
12	Modeling molecular recognition: theory and application. *Journal of Biomolecular Structure and Dynamics*, **2000**, 17 Suppl 1, 89-94	3.6	3
11	Molecular Basis for Polyketide Ketoreductase-Substrate Interactions. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	3
10	Leveraging Oxidative Stress to Regulate Redox Balance-Based, Growth Selections for Oxygenase Engineering. *ACS Synthetic Biology*, **2020**, 9, 3124-3133	5.7	3
9	Estimating the Roles of Protonation and Electronic Polarization in Absolute Binding Affinity Simulations. *Journal of Chemical Theory and Computation*, **2021**, 17, 2541-2555	6.4	3
8	The Hippo pathway kinases LATS1 and LATS2 attenuate cellular responses to heavy metals through phosphorylating MTF1.. *Nature Cell Biology*, **2022**, 24, 74-87	23.4	1
7	In Vivo, High-Throughput Selection of Thermostable Cyclohexanone Monooxygenase (CHMO). *Catalysts*, **2020**, 10, 935	4	1
6	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	5.7	1
5	Heparin-Assisted Amyloidogenesis Uncovered through Molecular Dynamics Simulations.. *ACS Omega*, **2022**, 7, 15132-15144	3.9	1
4	Development of a Pantetheine Force Field Library for Molecular Modeling. *Journal of Chemical Information and Modeling*, **2021**, 61, 856-868	6.1	0
3	Growth-Based, High-Throughput Selection for NADH Preference in an Oxygen-Dependent Biocatalyst. *ACS Synthetic Biology*, **2021**, 10, 2359-2370	5.7	0
2	Stress tensor and constant pressure simulation for polarizable Gaussian multipole model.. *Journal of Chemical Physics*, **2022**, 156, 114114	3.9	0

1	Machine-Learned Molecular Surface and Its Application to Implicit Solvent Simulations. *Journal of Chemical Theory and Computation*, **2021**, 17, 6214-6224	6.4