Benzhuo Lu

List of Publications by Year
in descending order

74	1,945	279701 23	265120 42
papers	citations	h-index	g-index

74	74	74	1557
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Computational Analysis and Prediction of the Binding Motif and Protein Interacting Partners of the Abl SH3 Domain. PLoS Computational Biology, 2006, 2, e1.	1.5	145
2	Order N algorithm for computation of electrostatic interactions in biomolecular systems. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 19314-19319.	3.3	129
3	Poissonâ€“Nernstâ€“Planck equations for simulating biomolecular diffusionâ€“reaction processes I: Finite element solutions. Journal of Computational Physics, 2010, 229, 6979-6994.	1.9	119
4	Poisson-Nernst-Planck Equations for Simulating Biomolecular Diffusion-Reaction Processes II: Size Effects on Ionic Distributions andÂDiffusion-Reaction Rates. Biophysical Journal, 2011, 100, 2475-2485.	0.2	108
5	Channel Opening Motion of Î±7 Nicotinic Acetylcholine Receptor as Suggested by Normal Mode Analysis. Journal of Molecular Biology, 2006, 355, 310-324.	2.0	104
6	Computation of electrostatic forces between solvated molecules determined by the Poissonâ€“Boltzmann equation using a boundary element method. Journal of Chemical Physics, 2005, 122, 214102.	1.2	95
7	Electrodiffusion: A continuum modeling framework for biomolecular systems with realistic spatiotemporal resolution. Journal of Chemical Physics, 2007, 127, 135102.	1.2	77
8	Improved Ion Transport and High Energy Conversion through Hydrogel Membrane with 3D Interconnected Nanopores. Nano Letters, 2020, 20, 5705-5713.	4.5	71
9	Prediction of Binding Affinities between the Human Amphiphysin-1 SH3 Domain and Its Peptide Ligands Using Homology Modeling, Molecular Dynamics and Molecular Field Analysis. Journal of Proteome Research, 2006, 5, 32-43.	1.8	70
10	Free Energy for the Permeation of Na⁺ and Cl^{â^'} Ions and Their Ion-Pair through a Zwitterionic Dimyristoyl Phosphatidylcholine Lipid Bilayer by Umbrella Integration with Harmonic Fourier Beads. Journal of the American Chemical Society, 2009, 131, 1706-1716.	6.6	70
11	TMSmesh: A Robust Method for Molecular Surface Mesh Generation Using a Trace Technique. Journal of Chemical Theory and Computation, 2011, 7, 203-212.	2.3	57
12	An Adaptive Fast Multipole Boundary Element Method for Poissonâ^'Boltzmann Electrostatics. Journal of Chemical Theory and Computation, 2009, 5, 1692-1699.	2.3	50
13	Improved Ion Transport in Hydrogel-Based Nanofluidics for Osmotic Energy Conversion. ACS Central Science, 2020, 6, 2097-2104.	5.3	49
14	AFMPB: An adaptive fast multipole Poissonâ€“Boltzmann solver for calculating electrostatics in biomolecular systems. Computer Physics Communications, 2010, 181, 1150-1160.	3.0	42
15	Charged porous asymmetric membrane for enhancing salinity gradient energy conversion. Nano Energy, 2021, 79, 105509.	8.2	42
16	Improved Boundary Element Methods for Poissonâ^'Boltzmann Electrostatic Potential and Force Calculations. Journal of Chemical Theory and Computation, 2007, 3, 1134-1142.	2.3	40
17	A parallel finite element simulator for ion transport through threeâ€dimensional ion channel systems. Journal of Computational Chemistry, 2013, 34, 2065-2078.	1.5	38
18	â€œNew-version-fast-multipole-methodâ€•accelerated electrostatic calculations in biomolecular systems. Journal of Computational Physics, 2007, 226, 1348-1366.	1.9	35

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19	Continuum Simulations of Acetylcholine Consumption by Acetylcholinesterase:â€‰ A Poissonâ^'Nernstâ^'Planck Approach. Journal of Physical Chemistry B, 2008, 112, 270-275.	1.2	34
20	Release of ADP from the catalytic subunit of protein kinase A: A molecular dynamics simulation study. Protein Science, 2009, 14, 159-168.	3.1	33
21	Triangulated manifold meshing method preserving molecular surface topology. Journal of Molecular Graphics and Modelling, 2012, 38, 411-418.	1.3	29
22	Direct estimation of entropy loss due to reduced translational and rotational motions upon molecular binding. Biopolymers, 2005, 79, 277-285.	1.2	26
23	Incorporating Born solvation energy into the three-dimensional Poisson-Nernst-Planck model to study ion selectivity in KcsA K+ channels. Physical Review E, 2017, 96, 062416.	0.8	25
24	Toward a Model for Activation of Orai Channel. IScience, 2019, 16, 356-367.	1.9	24
25	Enzymatic Activity versus Structural Dynamics: The Case of Acetylcholinesterase Tetramer. Biophysical Journal, 2009, 97, 897-905.	0.2	22
26	Ionic size effects to molecular solvation energy and to ion current across a channel resulted from the nonuniform size-modified PNP equations. Journal of Chemical Physics, 2014, 140, 174102.	1.2	22
27	Calculation of the Maxwell stress tensor and the Poisson-Boltzmann force on a solvated molecular surface using hypersingular boundary integrals. Journal of Chemical Physics, 2005, 123, 084904.	1.2	20
28	A Local Approximation of Fundamental Measure Theory Incorporated into Three Dimensional Poissonâ€“Nernstâ€“Planck Equations to Account for Hard Sphere Repulsion Among Ions. Journal of Statistical Physics, 2016, 163, 156-174.	0.5	20
29	An ionic concentration and size dependent dielectric permittivity Poisson-Boltzmann model for biomolecular solvation studies. Journal of Chemical Physics, 2014, 141, 024115.	1.2	19
30	Conic shapes have higher sensitivity than cylindrical ones in nanopore DNA sequencing. Scientific Reports, 2018, 8, 9097.	1.6	18
31	Parallel AFMPB solver with automatic surface meshing for calculation of molecular solvation free energy. Computer Physics Communications, 2015, 190, 173-181.	3.0	17
32	Modeling selective ion adsorption into cylindrical nanopores. Chemical Physics Letters, 2018, 709, 116-124.	1.2	17
33	Quality improvement of surface triangular mesh using a modified Laplacian smoothing approach avoiding intersection. PLoS ONE, 2017, 12, e0184206.	1.1	17
34	Stabilized finite element methods to simulate the conductances of ion channels. Computer Physics Communications, 2015, 188, 131-139.	3.0	16
35	E230Q mutation of the catalytic subunit of cAMP-dependent protein kinase affects local structure and the binding of peptide inhibitor. Biopolymers, 2006, 81, 428-439.	1.2	15
36	Molecular surface-free continuum model for electrodiffusion processes. Chemical Physics Letters, 2008, 451, 282-286.	1.2	15

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37	Solutions to a reduced Poissonâ€“Nernstâ€“Planck system and determination of reaction rates. Physica A: Statistical Mechanics and Its Applications, 2010, 389, 1329-1345.	1.2	15
38	Kinetics of diffusion-controlled enzymatic reactions with charged substrates. PMC Biophysics, 2010, 3, 1.	2.2	15
39	Efficient and Qualified Mesh Generation for Gaussian Molecular Surface Using Adaptive Partition and Piecewise Polynomial Approximation. SIAM Journal of Scientific Computing, 2018, 40, B507-B527.	1.3	15
40	Parameterization for molecular Gaussian surface and a comparison study of surface mesh generation. Journal of Molecular Modeling, 2015, 21, 113.	0.8	14
41	An Error Analysis for the Finite Element Approximation to the Steady-State Poisson-Nernst-Planck Equations. Advances in Applied Mathematics and Mechanics, 2013, 5, 113-130.	0.7	13
42	Mathematical and Numerical Aspects of the Adaptive Fast Multipole Poisson-Boltzmann Solver. Communications in Computational Physics, 2013, 13, 107-128.	0.7	12
43	Analysis of the Mean Field Free Energy Functional of Electrolyte Solution with Nonhomogenous Boundary Conditions and the Generalized PB/PNP Equations with Inhomogeneous Dielectric Permittivity. SIAM Journal on Applied Mathematics, 2018, 78, 1131-1154.	0.8	11
44	Parallel Adaptive Finite Element Algorithms for Solving the Coupled Electro-diffusion Equations. Computational and Mathematical Biophysics, 2013, 1, 90-108.	0.6	8
45	VCMM: A visual tool for continuum molecular modeling. Journal of Molecular Graphics and Modelling, 2014, 50, 44-49.	1.3	8
46	Molecular Surface Remeshing with Local Region Refinement. International Journal of Molecular Sciences, 2018, 19, 1383.	1.8	8
47	A decoupling two-grid method for the time-dependent Poisson-Nernst-Planck equations. Numerical Algorithms, 2020, 83, 1613-1651.	1.1	8
48	A stabilized finite element method for the Poissonâ€“Nernstâ€“Planck equations in three-dimensional ion channel simulations. Applied Mathematics Letters, 2021, 111, 106652.	1.5	8
49	A Finite Element Solution of Lateral Periodic Poissonâ€“Boltzmann Model for Membrane Channel Proteins. International Journal of Molecular Sciences, 2018, 19, 695.	1.8	7
50	Membrane-Channel Protein System Mesh Construction for Finite Element Simulations. Computational and Mathematical Biophysics, 2015, 3, .	0.6	6
51	A flux-jump preserved gradient recovery technique for accurately predicting the electrostatic field of an immersed biomolecule. Journal of Computational Physics, 2019, 396, 193-208.	1.9	6
52	An Effective Finite Element Iterative Solver for a Poisson--Nernst--Planck Ion Channel Model with Periodic Boundary Conditions. SIAM Journal of Scientific Computing, 2020, 42, B1490-B1516.	1.3	6
53	AFMPB: An adaptive fast multipole Poissonâ€“Boltzmann solver for calculating electrostatics in biomolecular systems. Computer Physics Communications, 2013, 184, 2618-2619.	3.0	5
54	Molecular Sparse Representation by a 3D Ellipsoid Radial Basis Function Neural Network via L1 Regularization. Journal of Chemical Information and Modeling, 2020, 60, 6054-6064.	2.5	5

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55	Advances in biomolecular surface meshing and its applications to mathematical modeling. Science Bulletin, 2013, 58, 1843-1849.	1.7	4
56	Charged Substrate and Product Together Contribute Like a Nonreactive Species to the Overall Electrostatic Steering in Diffusion-Reaction Processes. Journal of Physical Chemistry B, 2016, 120, 8147-8153.	1.2	4
57	A Time-Dependent Finite Element Algorithm for Simulations of Ion Current Rectification and Hysteresis Properties of 3D Nanopore System. IEEE Nanotechnology Magazine, 2018, 17, 513-519.	1.1	4
58	Model reduction-based initialization methods for solving the Poisson-Nernst-Plank equations in three-dimensional ion channel simulations. Journal of Computational Physics, 2020, 419, 109627.	1.9	4
59	A new block preconditioner and improved finite element solver of Poisson-Nernst-Planck equation. Journal of Computational Physics, 2021, 430, 110098.	1.9	4
60	The toolbox PHG and its applications. Scientia Sinica Informationis, 2016, 46, 1442-1464.	0.2	4
61	An effective sequence-alignment-free superpositioning of pairwise or multiple structures with missing data. Algorithms for Molecular Biology, 2016, 11, 18.	0.3	3
62	A Multi-Time-Step Finite Element Algorithm for 3-D Simulation of Coupled Drift-Diffusion Reaction Process in Total Ionizing Dose Effect. IEEE Transactions on Semiconductor Manufacturing, 2018, 31, 183-189.	1.4	3
63	Surface Triangular Mesh and Volume Tetrahedral Mesh Generations for Biomolecular Modeling. Lecture Notes in Computational Vision and Biomechanics, 2013, , 85-106.	0.5	2
64	Automated Parallel and Body-Fitted Mesh Generation in Finite Element Simulation of Macromolecular Systems. Communications in Computational Physics, 2016, 19, 582-602.	0.7	2
65	Introducing Membrane Transport Energy into the Design of Sustainable Chemicals against Cytotoxicity. ACS Sustainable Chemistry and Engineering, 2018, 6, 2055-2061.	3.2	2
66	Superconvergent gradient recovery for nonlinear Poisson-Nernst-Planck equations with applications to the ion channel problem. Advances in Computational Mathematics, 2020, 46, 1.	0.8	2
67	A structure-preserving finite element discretization for the time-dependent Nernst-Planck equation. Journal of Applied Mathematics and Computing, 2022, 68, 1545-1564.	1.2	2
68	A class of finite element methods with averaging techniques for solving the three-dimensional drift-diffusion model in semiconductor device simulations. Journal of Computational Physics, 2022, 458, 111086.	1.9	2
69	A Fast Direct Solver for a Class of 3-D Elliptic Partial Differential Equation with Variable Coefficient. Communications in Computational Physics, 2012, 12, 1148-1162.	0.7	1
70	Finite Element Modeling of Biomolecular Systems in Ionic Solution. Lecture Notes in Computational Vision and Biomechanics, 2013, , 271-301.	0.5	1
71	Residual Type a Posteriori Error Estimates for the Time-Dependent Poissonâ€“Nernstâ€“Planck Equations. Journal of Scientific Computing, 2022, 90, 1.	1.1	1
72	A Software Platform for Finite Element Simulation of Ion Permeation in Ion Channel Systems. Biophysical Journal, 2014, 106, 806a.	0.2	0

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73	An inverse averaging finite element method for solving three-dimensional Poisson-Nernst-Planck equations in nanopore system simulations. Journal of Chemical Physics, 2021, 155, 194106.	1.2	0
74	Poisson-Nernst-Planck Equation. , 2015, , 1159-1162.		0