BenoÄ±Ì‚t Roux

List of Publications by Year
in descending order

326 papers	44,917 citations	1713 107 h-index	2634 200 g-index
338 all docs	338 docs citations	338 times ranked	30713 citing authors

#	Article	IF	Citations
1	A Companion Guide to the String Method with Swarms of Trajectories: Characterization, Performance, and Pitfalls. Journal of Chemical Theory and Computation, 2022, 18, 1406-1422.	2.3	14
2	Challenges and Advantages of Accounting for Backbone Flexibility in Prediction of Proteinâ€“Protein Complexes. Journal of Chemical Theory and Computation, 2022, 18, 2016-2032.	2.3	2
3	Engineering of a synthetic antibody fragment for structural and functional studies of K+ channels. Journal of General Physiology, 2022, 154, .	0.9	0
4	A distinct mechanism of C-type inactivation in the Kv-like KcsA mutant E71V. Nature Communications, 2022, 13, 1574.	5.8	11
5	Accurate determination of protein:ligand standard binding free energies from molecular dynamics simulations. Nature Protocols, 2022, 17, 1114-1141.	5.5	56
6	Transition rate theory, spectral analysis, and reactive paths. Journal of Chemical Physics, 2022, 156, 134111.	1.2	20
7	Metal-responsive regulation of enzyme catalysis using genetically encoded chemical switches. Nature Communications, 2022, 13, 1864.	5.8	15
8	Hazardous Shortcuts in Standard Binding Free Energy Calculations. Journal of Physical Chemistry Letters, 2022, 13, 6250-6258.	2.1	10
9	Computational Assessment of Proteinâ€“Protein Binding Specificity within a Family of Synaptic Surface Receptors. Journal of Physical Chemistry B, 2022, 126, 7510-7527.	1.2	6
10	Molecular Dynamics Simulations Based on Polarizable Models Show that Ion Permeation Interconverts between Different Mechanisms as a Function of Membrane Thickness. Journal of Physical Chemistry B, 2021, 125, 1020-1035.	1.2	12
11	Polarization Effects in Water-Mediated Selective Cation Transport across a Narrow Transmembrane Channel. Journal of Chemical Theory and Computation, 2021, 17, 1726-1741.	2.3	26
12	A critical perspective on Markov state model treatments of proteinâ€“protein association using coarse-grained simulations. Journal of Chemical Physics, 2021, 154, 084101.	1.2	17
13	Elusive Intermediate State Key in the Conversion of ATP Hydrolysis into Useful Work Driving the Ca2+ Pump SERCA. Journal of Physical Chemistry B, 2021, 125, 2921-2928.	1.2	3
14	Classical molecular dynamics. Journal of Chemical Physics, 2021, 154, 100401.	1.2	28
15	Synthesis, Characterization, and Simulation of Four-Armed Megamolecules. Biomacromolecules, 2021, 22, 2363-2372.	2.6	4
16	Crystal structure of an archaeal CorB magnesium transporter. Nature Communications, 2021, 12, 4028.	5.8	23
17	Editorial: Advances in computational molecular biophysics. Biochimica Et Biophysica Acta - General Subjects, 2021, 1865, 129888.	1.1	0
18	The breakthrough of a quantum chemist by classical dynamics: Martin Karplus and the birth of computer simulations of chemical reactions. European Physical Journal H, 2021, 46, 1.	0.5	1

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19	Virtual Issue on Ion Channels and Ion Permeation. Journal of Physical Chemistry B, 2021, 125, 7575-7577.	1.2	1
20	String Method with Swarms-of-Trajectories, Mean Drifts, Lag Time, and Committor. Journal of Physical Chemistry A, 2021, 125, 7558-7571.	1.1	24
21	Engineering Dirhodium Artificial Metalloenzymes for Diazo Coupling Cascade Reactions**. Angewandte Chemie - International Edition, 2021, 60, 23672-23677.	7.2	10
22	Folding and misfolding of potassium channel monomers during assembly and tetramerization. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	5
23	Computational study of non-conductive selectivity filter conformations and C-type inactivation in a voltage-dependent potassium channel. Journal of General Physiology, 2021, 153, .	0.9	14
24	Computational Modeling and Simulations of Biomolecular Systems. , 2021, , .		6
25	Mechanism of C-type inactivation in the hERG potassium channel. Science Advances, 2021, 7, .	4.7	26
26	Frontispiz: Engineering Dirhodium Artificial Metalloenzymes for Diazo Coupling Cascade Reactions. Angewandte Chemie, 2021, 133, .	1.6	0
27	Global Optimization of the Lennard-Jones Parameters for the Drude Polarizable Force Field. Journal of Chemical Theory and Computation, 2021, 17, 7085-7095.	2.3	10
28	Tyrosine kinases: complex molecular systems challenging computational methodologies. European Physical Journal B, 2021, 94, 1.	0.6	3
29	Frontispiece: Engineering Dirhodium Artificial Metalloenzymes for Diazo Coupling Cascade Reactions. Angewandte Chemie - International Edition, 2021, 60, .	7.2	0
30	CHARMMâ€GUI DEER facilitator for spinâ€pair distance distribution calculations and preparation of restrainedâ€ensemble molecular dynamics simulations. Journal of Computational Chemistry, 2020, 41, 415-420.	1.5	19
31	Quantum Chemical Methods for Modeling Covalent Modification of Biological Thiols. Journal of Computational Chemistry, 2020, 41, 427-438.	1.5	31
32	Membrane Anchoring of Hck Kinase via the Intrinsically Disordered SH4-U and Length Scale Associated with Subcellular Localization. Journal of Molecular Biology, 2020, 432, 2985-2997.	2.0	10
33	Barium blockade of the KcsA channel in open and closed conformation datasets. Data in Brief, 2020, 32, 106135.	0.5	1
34	Open and Closed Structures of a Barium-Blocked Potassium Channel. Journal of Molecular Biology, 2020, 432, 4783-4798.	2.0	14
35	Continuum Electrostatic Behavior of a 3D-RISM Theory. Journal of Physical Chemistry B, 2020, 124, 7444-7451.	1.2	3
36	Identification of Druggable Kinase Target Conformations Using Markov Model Metastable States Analysis of apo-Abl. Journal of Chemical Theory and Computation, 2020, 16, 1896-1912.	2.3	16

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37	Scalable molecular dynamics on CPU and GPU architectures with NAMD. Journal of Chemical Physics, 2020, 153, 044130.	1.2	1,548
38	CHARMM-GUI Free Energy Calculator for Absolute and Relative Ligand Solvation and Binding Free Energy Simulations. Journal of Chemical Theory and Computation, 2020, 16, 7207-7218.	2.3	57
39	Statistical mechanics of polarizable force fields based on classical Drude oscillators with dynamical propagation by the dual-thermostat extended Lagrangian. Journal of Chemical Physics, 2020, 153, 114108.	1.2	11
40	Diversity of Long-Lived Intermediates along the Binding Pathway of Imatinib to Abl Kinase Revealed by MD Simulations. Journal of Chemical Theory and Computation, 2020, 16, 7852-7865.	2.3	14
41	pKa Calculations with the Polarizable Drude Force Field and Poissonâ€“Boltzmann Solvation Model. Journal of Chemical Theory and Computation, 2020, 16, 4655-4668.	2.3	14
42	Glycine substitution in SH3-SH2 connector of Hck tyrosine kinase causes population shift from assembled to disassembled state. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129604.	1.1	3
43	Characteristics of Impactful Computational Contributions to The Journal of Physical Chemistry B. Journal of Physical Chemistry B, 2020, 124, 5093-5094.	1.2	3
44	Further Optimization and Validation of the Classical Drude Polarizable Protein Force Field. Journal of Chemical Theory and Computation, 2020, 16, 3221-3239.	2.3	53
45	Biochemical patterns of antibody polyreactivity revealed through a bioinformatics-based analysis of CDR loops. ELife, 2020, 9, .	2.8	29
46	Computing Relative Binding Affinity of Ligands to Receptor: An Effective Hybrid Single-Dual-Topology Free-Energy Perturbation Approach in NAMD. Journal of Chemical Information and Modeling, 2019, 59, 3794-3802.	2.5	52
47	String Method for Proteinâ€“Protein Binding Free-Energy Calculations. Journal of Chemical Theory and Computation, 2019, 15, 5829-5844.	2.3	33
48	Molecular Dynamics Simulations of Ionic Liquids and Electrolytes Using Polarizable Force Fields. Chemical Reviews, 2019, 119, 7940-7995.	23.0	386
49	Crystal Structure and Conformational Dynamics of Pyrococcus furiosus Prolyl Oligopeptidase. Biochemistry, 2019, 58, 1616-1626.	1.2	19
50	Calculating the Effect of Membrane Thickness onÂthe Lifetime of the Gramicidin A Channel: AÂLandmark. Biophysical Journal, 2019, 117, 1779-1780.	0.2	0
51	Shifts in the selectivity filter dynamics cause modal gating in K+ channels. Nature Communications, 2019, 10, 123.	5.8	66
52	1H, 15N, and 13C resonance assignments of the intrinsically disordered SH4 and Unique domains of Hck. Biomolecular NMR Assignments, 2019, 13, 71-74.	0.4	3
53	Predicting the Conformational Variability of Abl Tyrosine Kinase using Molecular Dynamics Simulations and Markov State Models. Journal of Chemical Theory and Computation, 2018, 14, 2721-2732.	2.3	47
54	Polarizable Force Field for Molecular Ions Based on the Classical Drude Oscillator. Journal of Chemical Information and Modeling, 2018, 58, 993-1004.	2.5	45

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55	A Catalytically Disabled Double Mutant of Src Tyrosine Kinase Can Be Stabilized into an Active-Like Conformation. Journal of Molecular Biology, 2018, 430, 881-889.	2.0	10
56	Graphâ€“Theoretic Analysis of Monomethyl Phosphate Clustering in Ionic Solutions. Journal of Physical Chemistry B, 2018, 122, 1484-1494.	1.2	46
57	Enhanced configurational sampling with hybrid non-equilibrium molecular dynamicsâ€“Monte Carlo propagator. Journal of Chemical Physics, 2018, 148, 014101.	1.2	26
58	Optimized Lennard-Jones Parameters for Druglike Small Molecules. Journal of Chemical Theory and Computation, 2018, 14, 3121-3131.	2.3	44
59	Modeling induction phenomena in amino acid cationâ€“ $$pi $$ Ï€ interactions. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	14
60	Reproducibility of Free Energy Calculations across Different Molecular Simulation Software Packages. Journal of Chemical Theory and Computation, 2018, 14, 5567-5582.	2.3	66
61	Amphiphile-Induced Phase Transition of Liquid Crystals at Aqueous Interfaces. ACS Applied Materials & Interfaces, 2018, 10, 37618-37624.	4.0	23
62	Reduced Free Energy Perturbation/Hamiltonian Replica Exchange Molecular Dynamics Method with Unbiased Alchemical Thermodynamic Axis. Journal of Physical Chemistry B, 2018, 122, 9435-9442.	1.2	33
63	Proton Countertransport and Coupled Gating in the Sarcoplasmic Reticulum Calcium Pump. Journal of Molecular Biology, 2018, 430, 5050-5065.	2.0	15
64	Molecular Dynamics of Ion Conduction through the Selectivity Filter of the Na_VAb Sodium Channel. Journal of Physical Chemistry B, 2018, 122, 10126-10142.	1.2	26
65	Rapid constriction of the selectivity filter underlies C-type inactivation in the KcsA potassium channel. Journal of General Physiology, 2018, 150, 1408-1420.	0.9	64
66	Classical Drude Polarizable Force Field Model for Methyl Phosphate and Its Interactions with Mg²⁺. Journal of Physical Chemistry A, 2018, 122, 6147-6155.	1.1	23
67	A generalized linear response framework for expanded ensemble and replica exchange simulations. Journal of Chemical Physics, 2018, 149, 072315.	1.2	7
68	Combining the polarizable Drude force field with a continuum electrostatic Poissonâ€“Boltzmann implicit solvation model. Journal of Computational Chemistry, 2018, 39, 1707-1719.	1.5	15
69	Molecular Structure of Canonical Liquid Crystal Interfaces. Journal of the American Chemical Society, 2017, 139, 3841-3850.	6.6	56
70	Conformational Transitions and Alternating-Access Mechanism in the Sarcoplasmic Reticulum Calcium Pump. Journal of Molecular Biology, 2017, 429, 647-666.	2.0	37
71	Equivalence of M- and P-Summation in Calculations of Ionic Solvation Free Energies. Journal of Physical Chemistry A, 2017, 121, 1525-1530.	1.1	15
72	Inversion of the Sideâ€Chain Stereochemistry of Indvidual Thr or Ile Residues in a Protein Molecule: Impact on the Folding, Stability, and Structure of the ShK Toxin. Angewandte Chemie - International Edition, 2017, 56, 3324-3328.	7.2	17

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73	Perplexing cooperative folding and stability of a low-sequence complexity, polyproline 2 protein lacking a hydrophobic core. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 2241-2246.	3.3	29
74	Tyrosine Kinase Activation and Conformational Flexibility: Lessons from Src-Family Tyrosine Kinases. Accounts of Chemical Research, 2017, 50, 1193-1201.	7.6	53
75	Probing the Effects of Gating on the Ion Occupancy of the K⁺ Channel Selectivity Filter Using Two-Dimensional Infrared Spectroscopy. Journal of the American Chemical Society, 2017, 139, 8837-8845.	6.6	30
76	New Coarse Variables for the Accurate Determination of Standard Binding Free Energies. Journal of Chemical Theory and Computation, 2017, 13, 5173-5178.	2.3	49
77	Chemical substitutions in the selectivity filter of potassium channels do not rule out constricted-like conformations for C-type inactivation. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 11145-11150.	3.3	29
78	Drude Polarizable Force Field for Molecular Dynamics Simulations of Saturated and Unsaturated Zwitterionic Lipids. Journal of Chemical Theory and Computation, 2017, 13, 4535-4552.	2.3	90
79	Phosphoantigen-induced conformational change of butyrophilin 3A1 (BTN3A1) and its implication on VÎ³9VÎ´2 T cell activation. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E7311-E7320.	3.3	90
80	Machine Learning Force Field Parameters from Ab Initio Data. Journal of Chemical Theory and Computation, 2017, 13, 4492-4503.	2.3	105
81	Water Flux Induced Reorientation of Liquid Crystals. ACS Central Science, 2017, 3, 1345-1349.	5.3	9
82	Constant-pH Molecular Dynamics Simulations for Large Biomolecular Systems. Journal of Chemical Theory and Computation, 2017, 13, 5933-5944.	2.3	139
83	The Activation of c-Src Tyrosine Kinase: Conformational Transition Pathway and Free Energy Landscape. Journal of Physical Chemistry B, 2017, 121, 3352-3363.	1.2	41
84	CHARMMâ€GUI 10 years for biomolecular modeling and simulation. Journal of Computational Chemistry, 2017, 38, 1114-1124.	1.5	224
85	Understanding Atomic-Scale Behavior of Liquid Crystals at Aqueous Interfaces. Journal of Chemical Theory and Computation, 2017, 13, 237-244.	2.3	31
86	Ion channels and ion selectivity. Essays in Biochemistry, 2017, 61, 201-209.	2.1	85
87	The selectivity of the Na+/K+-pump is controlled by binding site protonation and self-correcting occlusion. ELife, 2016, 5, .	2.8	33
88	Concepts and protocols for electrostatic free energies. Molecular Simulation, 2016, 42, 1090-1101.	0.9	30
89	Efficiency in nonequilibrium molecular dynamics Monte Carlo simulations. Journal of Chemical Physics, 2016, 145, 134109.	1.2	15
90	Multiple Time-Step Dual-Hamiltonian Hybrid Molecular Dynamics â€“ Monte Carlo Canonical Propagation Algorithm. Journal of Chemical Theory and Computation, 2016, 12, 1449-1458.	2.3	9

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91	Computational study of the <scp>W</scp>260<scp>A</scp> activating mutant of <scp>S</scp>rc tyrosine kinase. Protein Science, 2016, 25, 219-230.	3.1	11
92	Transition path theory analysis of c-Src kinase activation. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 9193-9198.	3.3	67
93	Instantaneous ion configurations in the K ⁺ ion channel selectivity filter revealed by 2D IR spectroscopy. Science, 2016, 353, 1040-1044.	6.0	174
94	Leveraging the Information from Markov State Models To Improve the Convergence of Umbrella Sampling Simulations. Journal of Physical Chemistry B, 2016, 120, 8733-8742.	1.2	14
95	An Empirical Polarizable Force Field Based on the Classical Drude Oscillator Model: Development History and Recent Applications. Chemical Reviews, 2016, 116, 4983-5013.	23.0	434
96	Multi-ion free energy landscapes underscore the microscopic mechanism of ion selectivity in the KcsA channel. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1722-1732.	1.4	34
97	Atomic mutagenesis in ion channels with engineered stoichiometry. ELife, 2016, 5, .	2.8	23
98	Implementation of extended <scp>L</scp>agrangian dynamics in <scp>GROMACS</scp> for polarizable simulations using the classical <scp>D</scp>rude oscillator model. Journal of Computational Chemistry, 2015, 36, 1473-1479.	1.5	79
99	Structural Refinement of Proteins by Restrained Molecular Dynamics Simulations with Non-interacting Molecular Fragments. PLoS Computational Biology, 2015, 11, e1004368.	1.5	26
100	Insights into the molecular foundations of electrical excitation. Journal of Molecular Biology, 2015, 427, 1-2.	2.0	4
101	Simulating the Distance Distribution between Spin-Labels Attached to Proteins. Journal of Physical Chemistry B, 2015, 119, 3901-3911.	1.2	46
102	Representation of Ionâ€“Protein Interactions Using the Drude Polarizable Force-Field. Journal of Physical Chemistry B, 2015, 119, 9401-9416.	1.2	101
103	Computational Study of the â€œDFG-Flipâ€•Conformational Transition in c-Abl and c-Src Tyrosine Kinases. Journal of Physical Chemistry B, 2015, 119, 1443-1456.	1.2	56
104	A Structural Rearrangement of the Na+/K+-ATPase Traps Ouabain within the External Ion Permeation Pathway. Journal of Molecular Biology, 2015, 427, 1335-1344.	2.0	10
105	Generalized Metropolis acceptance criterion for hybrid non-equilibrium molecular dynamicsâ€”Monte Carlo simulations. Journal of Chemical Physics, 2015, 142, 024101.	1.2	21
106	Constant-pH Hybrid Nonequilibrium Molecular Dynamicsâ€“Monte Carlo Simulation Method. Journal of Chemical Theory and Computation, 2015, 11, 3919-3931.	2.3	82
107	Mechanism of potassium ion uptake by the Na+/K+-ATPase. Nature Communications, 2015, 6, 7622.	5.8	57
108	Enhanced Sampling of an Atomic Model with Hybrid Nonequilibrium Molecular Dynamicsâ€”Monte Carlo Simulations Guided by a Coarse-Grained Model. Journal of Chemical Theory and Computation, 2015, 11, 3572-3583.	2.3	18

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109	Efficient Determination of Free Energy Landscapes in Multiple Dimensions from Biased Umbrella Sampling Simulations Using Linear Regression. Journal of Chemical Theory and Computation, 2015, 11, 3523-3529.	2.3	23
110	Perspective on computational and structural aspects of kinase discovery from IPK2014. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2015, 1854, 1595-1604.	1.1	4
111	Efficient Determination of Relative Entropy Using Combined Temperature and Hamiltonian Replica-Exchange Molecular Dynamics. Journal of Chemical Theory and Computation, 2015, 11, 2234-2244.	2.3	11
112	Quantum Effects in Cation Interactions with First and Second Coordination Shell Ligands in Metalloproteins. Journal of Chemical Theory and Computation, 2015, 11, 4992-5001.	2.3	42
113	Dynamics transitions at the outer vestibule of the KcsA potassium channel during gating. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 1831-1836.	3.3	51
114	Achieving ergodic sampling using replica-exchange free-energy calculations. Molecular Simulation, 2014, 40, 218-228.	0.9	23
115	Conformational dynamics of ligand-dependent alternating access in LeuT. Nature Structural and Molecular Biology, 2014, 21, 472-479.	3.6	136
116	Exploring the Conformational Transitions of Biomolecular Systems Using a Simple Two-State Anisotropic Network Model. PLoS Computational Biology, 2014, 10, e1003521.	1.5	112
117	Escherichia coli Peptidoglycan Structure and Mechanics as Predicted by Atomic-Scale Simulations. PLoS Computational Biology, 2014, 10, e1003475.	1.5	92
118	Using multiscale preconditioning to accelerate the convergence of iterative molecular calculations. Journal of Chemical Physics, 2014, 140, 184114.	1.2	11
119	Efficient hybrid non-equilibrium molecular dynamics - Monte Carlo simulations with symmetric momentum reversal. Journal of Chemical Physics, 2014, 141, 114107.	1.2	20
120	Locking the Active Conformation of c-Src Kinase through the Phosphorylation of the Activation Loop. Journal of Molecular Biology, 2014, 426, 423-435.	2.0	74
121	Activation pathway of Src kinase reveals intermediate states as targets for drug design. Nature Communications, 2014, 5, 3397.	5.8	300
122	Structural mechanism of voltage-dependent gating in an isolated voltage-sensing domain. Nature Structural and Molecular Biology, 2014, 21, 244-252.	3.6	228
123	Permeation Redux: Thermodynamics and Kinetics of Ion Movement through Potassium Channels. Biophysical Journal, 2014, 106, 1859-1863.	0.2	30
124	Computational Study of Gleevec and G6G Reveals Molecular Determinants of Kinase Inhibitor Selectivity. Journal of the American Chemical Society, 2014, 136, 14753-14762.	6.6	41
125	Recent Advances in Polarizable Force Fields for Macromolecules: Microsecond Simulations of Proteins Using the Classical Drude Oscillator Model. Journal of Physical Chemistry Letters, 2014, 5, 3144-3150.	2.1	139
126	CHARMM-GUI PDB Manipulator for Advanced Modeling and Simulations of Proteins Containing Nonstandard Residues. Advances in Protein Chemistry and Structural Biology, 2014, 96, 235-265.	1.0	214

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127	Comparison between Mean Forces and Swarms-of-Trajectories String Methods. Journal of Chemical Theory and Computation, 2014, 10, 524-533.	2.3	38
128	Conformational cycle and ion-coupling mechanism of the Na ⁺ /hydantoin transporter Mhp1. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 14752-14757.	3.3	83
129	Nucleotide Regulation of the Structure and Dynamics of G-Actin. Biophysical Journal, 2014, 106, 1710-1720.	0.2	22
130	Quantitative Analysis of the Water Occupancy around the Selectivity Filter of a K⁺ Channel in Different Gating Modes. Journal of the American Chemical Society, 2014, 136, 2000-2007.	6.6	70
131	Generalized scalable multiple copy algorithms for molecular dynamics simulations in NAMD. Computer Physics Communications, 2014, 185, 908-916.	3.0	115
132	An Overview of Electrostatic Free Energy Computations for Solutions and Proteins. Journal of Chemical Theory and Computation, 2014, 10, 2690-2709.	2.3	118
133	Markov State and Diffusive Stochastic Models in Electron Spin Resonance. Advances in Experimental Medicine and Biology, 2014, 797, 115-138.	0.8	3
134	Automated Force Field Parameterization for Nonpolarizable and Polarizable Atomic Models Based on Ab Initio Target Data. Journal of Chemical Theory and Computation, 2013, 9, 3543-3556.	2.3	212
135	Efficient Determination of Proteinâ€“Protein Standard Binding Free Energies from First Principles. Journal of Chemical Theory and Computation, 2013, 9, 3789-3798.	2.3	188
136	Simulations of Anionic Lipid Membranes: Development of Interaction-Specific Ion Parameters and Validation Using NMR Data. Journal of Physical Chemistry B, 2013, 117, 10183-10192.	1.2	181
137	Recovery from slow inactivation in K+ channels is controlled by water molecules. Nature, 2013, 501, 121-124.	13.7	171
138	Computational Analysis of the Binding Specificity of Gleevec to Abl, c-Kit, Lck, and c-Src Tyrosine Kinases. Journal of the American Chemical Society, 2013, 135, 14741-14753.	6.6	49
139	Simulation study of ion pairing in concentrated aqueous salt solutions with a polarizable force field. Faraday Discussions, 2013, 160, 135-149.	1.6	102
140	Polarizable Force Field for Peptides and Proteins Based on the Classical Drude Oscillator. Journal of Chemical Theory and Computation, 2013, 9, 5430-5449.	2.3	329
141	A Structural Study of Ion Permeation in OmpF Porin from Anomalous X-ray Diffraction and Molecular Dynamics Simulations. Journal of the American Chemical Society, 2013, 135, 16561-16568.	6.6	23
142	A Polarizable Force Field of Dipalmitoylphosphatidylcholine Based on the Classical Drude Model for Molecular Dynamics Simulations of Lipids. Journal of Physical Chemistry B, 2013, 117, 9142-9160.	1.2	159
143	Kirkwood-Buff analysis of aqueous N-methylacetamide and acetamide solutions modeled by the CHARMM additive and Drude polarizable force fields. Journal of Chemical Physics, 2013, 139, 084509.	1.2	31
144	CHARMM-GUI Ligand Binder for Absolute Binding Free Energy Calculations and Its Application. Journal of Chemical Information and Modeling, 2013, 53, 267-277.	2.5	71

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145	The Binding of Antibiotics in OmpF Porin. Structure, 2013, 21, 76-87.	1.6	128
146	Eppur Si Muove! The 2013 Nobel Prize in Chemistry. Structure, 2013, 21, 2102-2105.	1.6	26
147	Six-site polarizable model of water based on the classical Drude oscillator. Journal of Chemical Physics, 2013, 138, 034508.	1.2	103
148	On the statistical equivalence of restrained-ensemble simulations with the maximum entropy method. Journal of Chemical Physics, 2013, 138, 084107.	1.2	166
149	The Theory of Ultra-Coarse-Graining. 1. General Principles. Journal of Chemical Theory and Computation, 2013, 9, 2466-2480.	2.3	149
150	Architecture and assembly of the <scp>G</scp>ramâ€positive cell wall. Molecular Microbiology, 2013, 88, 664-672.	1.2	116
151	Restrained-Ensemble Molecular Dynamics Simulations Based on Distance Histograms from Double Electronâ€“Electron Resonance Spectroscopy. Journal of Physical Chemistry B, 2013, 117, 4733-4739.	1.2	66
152	Self-Learning Adaptive Umbrella Sampling Method for the Determination of Free Energy Landscapes in Multiple Dimensions. Journal of Chemical Theory and Computation, 2013, 9, 1885-1895.	2.3	80
153	Standard Binding Free Energies from Computer Simulations: What Is the Best Strategy?. Journal of Chemical Theory and Computation, 2013, 9, 794-802.	2.3	298
154	Relative Free Energies for Hydration of Monovalent Ions from QM and QM/MM Simulations. Journal of Chemical Theory and Computation, 2013, 9, 4165-4175.	2.3	54
155	Structural Refinement from Restrained-Ensemble Simulations Based on EPR/DEER Data: Application to T4 Lysozyme. Journal of Physical Chemistry B, 2013, 117, 4740-4754.	1.2	88
156	QM/MM molecular dynamics simulations of the hydration of Mg(II) and Zn(II) ions. Canadian Journal of Chemistry, 2013, 91, 552-558.	0.6	36
157	A computational study of barium blockades in the KcsA potassium channel based on multi-ion potential of mean force calculations and free energy perturbation. Journal of General Physiology, 2013, 142, 451-463.	0.9	16
158	Molecular dynamics simulations of membrane proteins under asymmetric ionic concentrations. Journal of General Physiology, 2013, 142, 465-475.	0.9	51
159	Explaining why Gleevec is a specific and potent inhibitor of Abl kinase. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 1664-1669.	3.3	136
160	An emerging consensus on voltage-dependent gating from computational modeling and molecular dynamics simulations. Journal of General Physiology, 2012, 140, 587-594.	0.9	179
161	Intermediate state trapping of a voltage sensor. Journal of General Physiology, 2012, 140, 635-652.	0.9	50
162	Ion Binding Sites and Their Representations by Reduced Models. Journal of Physical Chemistry B, 2012, 116, 6966-6979.	1.2	16

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163	Comment on â€œProbing the Thermodynamics of Competitive Ion Binding Using Minimum Energy Structuresâ€. Journal of Physical Chemistry B, 2012, 116, 7991-7993.	1.2	1
164	Constant electric field simulations of the membrane potential illustrated with simple systems. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 294-302.	1.4	169
165	The Solvation Structure of Na⁺ and K⁺ in Liquid Water Determined from High Level ab Initio Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2012, 8, 3526-3535.	2.3	191
166	Multi-Ion Distributions in the Cytoplasmic Domain of Inward Rectifier Potassium Channels. Biophysical Journal, 2012, 103, 434-443.	0.2	7
167	Nano-Positioning System for Structural Analysis of Functional Homomeric Proteins in Multiple Conformations. Structure, 2012, 20, 1629-1640.	1.6	15
168	Calculation of Free Energy Landscape in Multi-Dimensions with Hamiltonian-Exchange Umbrella Sampling on Petascale Supercomputer. Journal of Chemical Theory and Computation, 2012, 8, 4672-4680.	2.3	89
169	Molecular Mechanisms of K+ Selectivity in Na/K Pump. Australian Journal of Chemistry, 2012, 65, 448.	0.5	6
170	Web interface for brownian dynamics simulation of ion transport and its applications to betaâ€barrel pores. Journal of Computational Chemistry, 2012, 33, 331-339.	1.5	43
171	Voltage-Gated Ion Channels: The Machines Responsible for the Nerve Impulse. , 2011, , 231-248.		1
172	Gramicidin A Backbone and Side Chain Dynamics Evaluated by Molecular Dynamics Simulations and Nuclear Magnetic Resonance Experiments. I: Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2011, 115, 7417-7426.	1.2	31
173	Computational Electrophysiology: The Molecular Dynamics of Ion Channel Permeation and Selectivity in Atomistic Detail. Biophysical Journal, 2011, 101, 755-756.	0.2	4
174	In Search of a Consensus Model of the Resting State of a Voltage-Sensing Domain. Neuron, 2011, 72, 713-720.	3.8	93
175	High-Performance Scalable Molecular Dynamics Simulations of a Polarizable Force Field Based on Classical Drude Oscillators in NAMD. Journal of Physical Chemistry Letters, 2011, 2, 87-92.	2.1	233
176	Thermodynamic coupling between activation and inactivation gating in potassium channels revealed by free energy molecular dynamics simulations. Journal of General Physiology, 2011, 138, 571-580.	0.9	49
177	On the structural basis of modal gating behavior in K+ channels. Nature Structural and Molecular Biology, 2011, 18, 67-74.	3.6	71
178	Computer simulations of water flux and salt permeability of the reverse osmosis FT-30 aromatic polyamide membrane. Journal of Membrane Science, 2011, 384, 1-9.	4.1	87
179	Ouabain Binding Site in a Functioning Na+/K+ ATPase. Journal of Biological Chemistry, 2011, 286, 38177-38183.	1.6	50
180	Biogenesis of the pore architecture of a voltage-gated potassium channel. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 3240-3245.	3.3	27

#	Article	IF	Citations
181	Ion selectivity in channels and transporters. Journal of General Physiology, 2011, 137, 415-426.	0.9	142
182	Protonation of key acidic residues is critical for the K+-selectivity of the Na/K pump. Nature Structural and Molecular Biology, 2011, 18, 1159-1163.	3.6	54
183	Simulation of Osmotic Pressure in Concentrated Aqueous Salt Solutions. Journal of Physical Chemistry Letters, 2010, 1, 183-189.	2.1	266
184	Calculation of the standard binding free energy of sparsomycin to the ribosomal peptidylâ€transferase Pâ€site using molecular dynamics simulations with restraining potentials. Journal of Molecular Recognition, 2010, 23, 128-141.	1.1	16
185	Structural basis for the coupling between activation and inactivation gates in K+ channels. Nature, 2010, 466, 272-275.	13.7	267
186	Perspectives on: Molecular dynamics and computational methods. Journal of General Physiology, 2010, 135, 547-548.	0.9	13
187	Two mechanisms of ion selectivity in protein binding sites. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 20329-20334.	3.3	83
188	The activated state of a sodium channel voltage sensor in a membrane environment. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 5435-5440.	3.3	46
189	Selectivity of externally facing ion-binding sites in the Na/K pump to alkali metals and organic cations. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 18718-18723.	3.3	31
190	Multidomain assembled states of Hck tyrosine kinase in solution. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 15757-15762.	3.3	195
191	Assessing the accuracy of approximate treatments of ion hydration based on primitive quasichemical theory. Journal of Chemical Physics, 2010, 132, 234101.	1.2	24
192	Calculation of the Gating Charge for the Kv1.2 Voltage-Activated Potassium Channel. Biophysical Journal, 2010, 98, 2189-2198.	0.2	135
193	Exploring the Ion Selectivity Properties of a Large Number of Simplified Binding Site Models. Biophysical Journal, 2010, 98, 2877-2885.	0.2	29
194	Absolute Binding Free Energy Calculations of Sparsomycin Analogs to the Bacterial Ribosome. Journal of Physical Chemistry B, 2010, 114, 9525-9539.	1.2	50
195	Ion Selectivity of Î±-Hemolysin with a Î²-Cyclodextrin Adapter. I. Single Ion Potential of Mean Force and Diffusion Coefficient. Journal of Physical Chemistry B, 2010, 114, 952-958.	1.2	37
196	Energetics of Double-Ion Occupancy in the Gramicidin A Channel. Journal of Physical Chemistry B, 2010, 114, 13881-13888.	1.2	15
197	Cation-selective Pathway of OmpF Porin Revealed by Anomalous X-ray Diffraction. Journal of Molecular Biology, 2010, 396, 293-300.	2.0	29
198	Ion Selectivity of the KcsA Channel: A Perspective from Multi-Ion Free Energy Landscapes. Journal of Molecular Biology, 2010, 401, 831-842.	2.0	90

#	Article	IF	Citations
199	Free Energy Perturbation Hamiltonian Replica-Exchange Molecular Dynamics (FEP/H-REMD) for Absolute Ligand Binding Free Energy Calculations. Journal of Chemical Theory and Computation, 2010, 6, 2559-2565.	2.3	211
200	Simulating Monovalent and Divalent Ions in Aqueous Solution Using a Drude Polarizable Force Field. Journal of Chemical Theory and Computation, 2010, 6, 774-786.	2.3	401
201	Accurate Calculation of Hydration Free Energies using Pair-Specific Lennard-Jones Parameters in the CHARMM Drude Polarizable Force Field. Journal of Chemical Theory and Computation, 2010, 6, 1181-1198.	2.3	131
202	Perspectives on: Molecular dynamics and computational methods. Journal of Cell Biology, 2010, 189, i16-i16.	2.3	0
203	Mapping the conformational transition in Src activation by cumulating the information from multiple molecular dynamics trajectories. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 3776-3781.	3.3	106
204	CHARMM: The biomolecular simulation program. Journal of Computational Chemistry, 2009, 30, 1545-1614.	1.5	7,077
205	Molecular modeling and dynamics studies with explicit inclusion of electronic polarizability: theory and applications. Theoretical Chemistry Accounts, 2009, 124, 11-28.	0.5	314
206	Binding specificity of SH2 domains: Insight from free energy simulations. Proteins: Structure, Function and Bioinformatics, 2009, 74, 996-1007.	1.5	46
207	Computations of Standard Binding Free Energies with Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 2234-2246.	1.2	481
208	Hydration Number, Topological Control, and Ion Selectivity. Journal of Physical Chemistry B, 2009, 113, 8725-8730.	1.2	34
209	Free Energy and Kinetics of Conformational Transitions from Voronoi Tessellated Milestoning with Restraining Potentials. Journal of Chemical Theory and Computation, 2009, 5, 2589-2594.	2.3	62
210	Computation of Absolute Hydration and Binding Free Energy with Free Energy Perturbation Distributed Replica-Exchange Molecular Dynamics. Journal of Chemical Theory and Computation, 2009, 5, 2583-2588.	2.3	120
211	A Rapid Coarse Residue-Based Computational Method for X-Ray Solution Scattering Characterization of Protein Folds and Multiple Conformational States of Large Protein Complexes. Biophysical Journal, 2009, 96, 4449-4463.	0.2	117
212	Atomistic View of the Conformational Activation of Src Kinase Using the String Method with Swarms-of-Trajectories. Biophysical Journal, 2009, 97, L8-L10.	0.2	84
213	On the Utilization of Energy Minimization to the Study of Ion Selectivity. Biophysical Journal, 2009, 97, L15-L17.	0.2	17
214	Molecular Dynamics Study of a Polymeric Reverse Osmosis Membrane. Journal of Physical Chemistry B, 2009, 113, 10177-10182.	1.2	139
215	Multifrequency Electron Spin Resonance Spectra of a Spin-Labeled Protein Calculated from Molecular Dynamics Simulations. Journal of the American Chemical Society, 2009, 131, 2597-2605.	6.6	73
216	Many-Body Polarization Effects and the Membrane Dipole Potential. Journal of the American Chemical Society, 2009, 131, 2760-2761.	6.6	98

#	Article	IF	Citations
217	Computations of Absolute Solvation Free Energies of Small Molecules Using Explicit and Implicit Solvent Model. Journal of Chemical Theory and Computation, 2009, 5, 919-930.	2.3	136
218	Flexibility and charge asymmetry in the activation loop of Src tyrosine kinases. Proteins: Structure, Function and Bioinformatics, 2009, 74, 378-389.	1.5	38
219	Computation of binding free energy with molecular dynamics and grand canonical Monte Carlo simulations. Journal of Chemical Physics, 2008, 128, 115103.	1.2	123
220	Structural Refinement of Membrane Proteins by Restrained Molecular Dynamics and Solvent Accessibility Data. Biophysical Journal, 2008, 95, 5349-5361.	0.2	23
221	Parametrization, Molecular Dynamics Simulation, and Calculation of Electron Spin Resonance Spectra of a Nitroxide Spin Label on a Polyalanine Î±-Helix. Journal of Physical Chemistry B, 2008, 112, 5755-5767.	1.2	98
222	Control of Ion Selectivity in LeuT: Two Na+ Binding Sites with Two Different Mechanisms. Journal of Molecular Biology, 2008, 377, 804-818.	2.0	181
223	On the origin of the electrostatic potential difference at a liquid-vacuum interface. Journal of Chemical Physics, 2008, 129, 234706.	1.2	88
224	The Membrane Potential and its Representation by a Constant Electric Field in Computer Simulations. Biophysical Journal, 2008, 95, 4205-4216.	0.2	188
225	Understanding the Dielectric Properties of Liquid Amides from a Polarizable Force Field. Journal of Physical Chemistry B, 2008, 112, 3509-3521.	1.2	122
226	Finding Transition Pathways Using the String Method with Swarms of Trajectories. Journal of Physical Chemistry B, 2008, 112, 3432-3440.	1.2	313
227	Building Markov state models along pathways to determine free energies and rates of transitions. Journal of Chemical Physics, 2008, 129, 064107.	1.2	137
228	Comment on â€œFree energy simulations of single and double ion occupancy in gramicidin Aâ€•[J. Chem. Phys. 126, 105103 (2007)]. Journal of Chemical Physics, 2008, 128, 227101.	1.2	21
229	Src Kinase Conformational Activation: Thermodynamics, Pathways, and Mechanisms. PLoS Computational Biology, 2008, 4, e1000047.	1.5	91
230	Long-pore Electrostatics in Inward-rectifier Potassium Channels. Journal of General Physiology, 2008, 132, 613-632.	0.9	46
231	What Can Be Deduced about the Structure of Shaker from Available Data?. Novartis Foundation Symposium, 2008, , 84-108.	1.2	6
232	Importance of Hydration and Dynamics on the Selectivity of the KcsA and NaK Channels. Journal of General Physiology, 2007, 129, 135-143.	0.9	178
233	On the importance of a funneled energy landscape for the assembly and regulation of multidomain Src tyrosine kinases. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 13643-13648.	3.3	54
234	Closing In on the Resting State of the Shaker K+ Channel. Neuron, 2007, 56, 124-140.	3.8	270

#	Article	IF	Citations
235	Mechanism of Intracellular Block of the KcsA K+ Channel by Tetrabutylammonium: Insights from X-ray Crystallography, Electrophysiology and Replica-exchange Molecular Dynamics Simulations. Journal of Molecular Biology, 2007, 365, 649-662.	2.0	57
236	Two atomic constraints unambiguously position the S4 segment relative to S1 and S2 segments in the closed state of Shaker K channel. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 7904-7909.	3.3	164
237	Polarizable Empirical Force Field for Aromatic Compounds Based on the Classical Drude Oscillator. Journal of Physical Chemistry B, 2007, 111, 2873-2885.	1.2	149
238	Theoretical Study of Aqueous Solvation of K⁺ Comparing ab Initio, Polarizable, and Fixed-Charge Models. Journal of Chemical Theory and Computation, 2007, 3, 2068-2082.	2.3	87
239	Dynamics of the Kv1.2 Voltage-Gated K+ Channel in a Membrane Environment. Biophysical Journal, 2007, 93, 3070-3082.	0.2	138
240	Polarizable Empirical Force Field for the Primary and Secondary Alcohol Series Based on the Classical Drude Model. Journal of Chemical Theory and Computation, 2007, 3, 1927-1946.	2.3	136
241	Characterization of conformational equilibria through Hamiltonian and temperature replica-exchange simulations: Assessing entropic and environmental effects. Journal of Computational Chemistry, 2007, 28, 1634-1647.	1.5	44
242	Anatomy of a structural pathway for activation of the catalytic domain of Src kinase Hck. Proteins: Structure, Function and Bioinformatics, 2007, 67, 1096-1112.	1.5	39
243	A proton-controlled check valve for sodium ion transport. Nature Chemical Biology, 2007, 3, 609-610.	3.9	2
244	Molecular driving forces determining potassium channel slow inactivation. Nature Structural and Molecular Biology, 2007, 14, 1062-1069.	3.6	216
245	Calculation of Standard Binding Free Energies:â€‰ Aromatic Molecules in the T4 Lysozyme L99A Mutant. Journal of Chemical Theory and Computation, 2006, 2, 1255-1273.	2.3	265
246	Ion Permeation through a Narrow Channel: Using Gramicidin to Ascertain All-Atom Molecular Dynamics Potential of Mean Force Methodology and Biomolecular Force Fields. Biophysical Journal, 2006, 90, 3447-3468.	0.2	133
247	Absolute Binding Free Energy Calculations Using Molecular Dynamics Simulations with Restraining Potentials. Biophysical Journal, 2006, 91, 2798-2814.	0.2	316
248	Atomic Level Anisotropy in the Electrostatic Modeling of Lone Pairs for a Polarizable Force Field Based on the Classical Drude Oscillator. Journal of Chemical Theory and Computation, 2006, 2, 1587-1597.	2.3	142
249	Absolute Hydration Free Energy Scale for Alkali and Halide Ions Established from Simulations with a Polarizable Force Field. Journal of Physical Chemistry B, 2006, 110, 3308-3322.	1.2	357
250	Dissecting the Coupling between the Voltage Sensor and Pore Domains. Neuron, 2006, 52, 568-569.	3.8	10
251	S3h1-1 Molecular Determinants of Gating at the K^+ Channel Selectivity Filter, Probed by Protein Crystallography and Molecular Dynamics Simulations(S3-h1: "Structural Aspects of Channel and) Tj ETQq1 1 0.784314 rgBT /Overlock 46, S139.	0.0	0
252	Molecular determinants of gating at the potassium-channel selectivity filter. Nature Structural and Molecular Biology, 2006, 13, 311-318.	3.6	399

#	Article	IF	Citations
253	Molecular dynamics â€" potential of mean force calculations as a tool for understanding ion permeation and selectivity in narrow channels. Biophysical Chemistry, 2006, 124, 251-267.	1.5	181
254	Ion selectivity in potassium channels. Biophysical Chemistry, 2006, 124, 279-291.	1.5	174
255	A polarizable model of water for molecular dynamics simulations of biomolecules. Chemical Physics Letters, 2006, 418, 245-249.	1.2	548
256	Extracellular Blockade of Potassium Channels by TEA+: The Tip of the Iceberg?. Journal of General Physiology, 2006, 128, 635-636.	0.9	4
257	Gating charge displacement in voltage-gated ion channels involves limited transmembrane movement. Nature, 2005, 436, 852-856.	13.7	263
258	A Gate in the Selectivity Filter of Potassium Channels. Structure, 2005, 13, 591-600.	1.6	190
259	The N-Terminal End of the Catalytic Domain of Src Kinase Hck Is a Conformational Switch Implicated in Long-Range Allosteric Regulation. Structure, 2005, 13, 1715-1723.	1.6	45
260	A Variable Residue in the Pore of Kv1 Channels Is Critical for the High Affinity of Blockers from Sea Anemones and Scorpions. Journal of Biological Chemistry, 2005, 280, 27093-27102.	1.6	42
261	Ion Conduction and Selectivity in K+ Channels. Annual Review of Biophysics and Biomolecular Structure, 2005, 34, 153-171.	18.3	167
262	Determination of Electrostatic Parameters for a Polarizable Force Field Based on the Classical Drude Oscillator. Journal of Chemical Theory and Computation, 2005, 1, 153-168.	2.3	260
263	Calculation of absolute protein-ligand binding free energy from computer simulations. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6825-6830.	3.3	594
264	Free Energy Landscape of A-DNA to B-DNA Conversion in Aqueous Solution. Journal of the American Chemical Society, 2005, 127, 6866-6876.	6.6	122
265	Electrostatics of the Intracellular Vestibule of K+ Channels. Journal of Molecular Biology, 2005, 354, 272-288.	2.0	58
266	The Art of Dissecting the Function of a Potassium Channel. Neuron, 2005, 47, 777-778.	3.8	5
267	Rapid Intracellular TEA Block of the KcsA Potassium Channel. Biophysical Journal, 2005, 88, 1018-1029.	0.2	48
268	Grand canonical Monte Carlo simulations of water in protein environments. Journal of Chemical Physics, 2004, 121, 6392-6400.	1.2	112
269	Energetics of ion conduction through the gramicidin channel. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 117-122.	3.3	371
270	Theoretical and computational models of biological ion channels. Quarterly Reviews of Biophysics, 2004, 37, 15-103.	2.4	362

#	Article	IF	Citations
271	Control of ion selectivity in potassium channels by electrostatic and dynamic properties of carbonyl ligands. Nature, 2004, 431, 830-834.	13.7	528
272	Computational Studies of Membrane Channels. Structure, 2004, 12, 1343-1351.	1.6	136
273	Critical assessment of a proposed model of Shaker. FEBS Letters, 2004, 564, 257-263.	1.3	35
274	Hydration of Amino Acid Side Chains:Â Nonpolar and Electrostatic Contributions Calculated from Staged Molecular Dynamics Free Energy Simulations with Explicit Water Molecules. Journal of Physical Chemistry B, 2004, 108, 16567-16576.	1.2	206
275	On the Importance of Atomic Fluctuations, Protein Flexibility, and Solvent in Ion Permeation. Journal of General Physiology, 2004, 124, 679-690.	0.9	141
276	Structure of Gramicidin A in a Lipid Bilayer Environment Determined Using Molecular Dynamics Simulations and Solid-State NMR Data. Journal of the American Chemical Society, 2003, 125, 9868-9877.	6.6	123
277	A simple polarizable model of water based on classical Drude oscillators. Journal of Chemical Physics, 2003, 119, 5185-5197.	1.2	635
278	Modeling induced polarization with classical Drude oscillators: Theory and molecular dynamics simulation algorithm. Journal of Chemical Physics, 2003, 119, 3025-3039.	1.2	584
279	A microscopic view of ion conduction through the K+ channel. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 8644-8648.	3.3	222
280	Atomic Radii for Continuum Electrostatics Calculations on Nucleic Acids. Journal of Physical Chemistry B, 2002, 106, 11026-11035.	1.2	69
281	Computational Studies of the Gramicidin Channel. Accounts of Chemical Research, 2002, 35, 366-375.	7.6	131
282	Electrostatic free energy calculations using the generalized solvent boundary potential method. Journal of Chemical Physics, 2002, 117, 7381-7388.	1.2	37
283	Ions and Counterions in a Biological Channel: A Molecular Dynamics Simulation of OmpF Porin from Escherichia coli in an Explicit Membrane with 1M KCl Aqueous Salt Solution. Journal of Molecular Biology, 2002, 319, 1177-1197.	2.0	252
284	Ion Permeation and Selectivity of OmpF Porin: A Theoretical Study Based on Molecular Dynamics, Brownian Dynamics, and Continuum Electrodiffusion Theory. Journal of Molecular Biology, 2002, 322, 851-869.	2.0	353
285	Modeling the Structure of Agitoxin in Complex with the Shaker K+ Channel: A Computational Approach Based on Experimental Distance Restraints Extracted from Thermodynamic Mutant Cycles. Biophysical Journal, 2002, 83, 2595-2609.	0.2	124
286	On the Potential Functions used in Molecular Dynamics Simulations of Ion Channels. Biophysical Journal, 2002, 82, 1681-1684.	0.2	76
287	Molecular Mechanism of H+ Conduction in the Single-File Water Chain of the Gramicidin Channel. Biophysical Journal, 2002, 82, 2304-2316.	0.2	250
288	What can be deduced about the structure of Shaker from available data?. Novartis Foundation Symposium, 2002, 245, 84-101; discussion 101-8, 165-8.	1.2	4

#	Article	IF	Citations
289	Generalized solvent boundary potential for computer simulations. Journal of Chemical Physics, 2001, 114, 2924-2937.	1.2	223
290	Lipid-Mediated Interactions between Intrinsic Membrane Proteins: Dependence on Protein Size and Lipid Composition. Biophysical Journal, 2001, 81, 276-284.	0.2	82
291	Dynamic Coupling between the SH2 and SH3 Domains of c-Src and Hck Underlies Their Inactivation by C-Terminal Tyrosine Phosphorylation. Cell, 2001, 105, 115-126.	13.5	366
292	Extension to the weighted histogram analysis method: combining umbrella sampling with free energy calculations. Computer Physics Communications, 2001, 135, 40-57.	3.0	816
293	Energetics of ion conduction through the K+ channel. Nature, 2001, 414, 73-77.	13.7	745
294	Extracellular Blockade of K+ Channels by Tea. Journal of General Physiology, 2001, 118, 207-218.	0.9	71
295	Brownian dynamics simulations of ions channels: A general treatment of electrostatic reaction fields for molecular pores of arbitrary geometry. Journal of Chemical Physics, 2001, 115, 4850-4861.	1.2	69
296	Anchoring of a monotopic membrane protein: the binding of prostaglandin H2 synthase-1 to the surface of a phospholipid bilayer. European Biophysics Journal, 2000, 29, 439-454.	1.2	49
297	A Grand Canonical Monte Carloâ€“Brownian Dynamics Algorithm for Simulating Ion Channels. Biophysical Journal, 2000, 79, 788-801.	0.2	226
298	Molecular Dynamics of the KcsA K+ Channel in a Bilayer Membrane. Biophysical Journal, 2000, 78, 2900-2917.	0.2	314
299	Solvation Free Energy of Polar and Nonpolar Molecules in Water:â€‰ An Extended Interaction Site Integral Equation Theory in Three Dimensions. Journal of Physical Chemistry B, 2000, 104, 796-805.	1.2	132
300	Free Energy Simulations:â€‰ Thermodynamic Reversibility and Variability. Journal of Physical Chemistry B, 2000, 104, 5179-5190.	1.2	32
301	Ion Channels, Permeation, and Electrostatics: Insight into the Function of KcsA. Biochemistry, 2000, 39, 13295-13306.	1.2	167
302	Implicit solvent models. Biophysical Chemistry, 1999, 78, 1-20.	1.5	793
303	Efficient calculation of two-dimensional adiabatic and free energy maps: Application to the isomerization of the C13?C14 and C15?N16 bonds in the retinal of bacteriorhodopsin. Journal of Computational Chemistry, 1999, 20, 1644-1658.	1.5	28
304	Statistical Mechanical Equilibrium Theory of Selective Ion Channels. Biophysical Journal, 1999, 77, 139-153.	0.2	130
305	The Binding Site of Sodium in the Gramicidin A Channel. Novartis Foundation Symposium, 1999, 225, 113-127.	1.2	2
306	Continuum solvation model: Computation of electrostatic forces from numerical solutions to the Poisson-Boltzmann equation. Computer Physics Communications, 1998, 111, 59-75.	3.0	500

#	Article	IF	Citations
307	Quantum Chemical and Free Energy Simulation Analysis of Retinal Conformational Energetics. Journal of Chemical Information and Computer Sciences, 1997, 37, 1018-1024.	2.8	30
308	An Integral Equation To Describe the Solvation of Polar Molecules in Liquid Water. Journal of Physical Chemistry B, 1997, 101, 7821-7826.	1.2	465
309	Atomic Radii for Continuum Electrostatics Calculations Based on Molecular Dynamics Free Energy Simulations. Journal of Physical Chemistry B, 1997, 101, 5239-5248.	1.2	369
310	A potential function for computer simulation studies of proton transfer in acetylacetone. Journal of Computational Chemistry, 1997, 18, 368-380.	1.5	43
311	Solvation of complex molecules in a polar liquid: An integral equation theory. Journal of Chemical Physics, 1996, 104, 8678-8689.	1.2	168
312	Structure, energetics, and dynamics of lipidâ€“protein interactions: A molecular dynamics study of the gramicidin A channel in a DMPC bilayer. , 1996, 24, 92-114.		274
313	Structure, energetics, and dynamics of lipidâ€“protein interactions: A molecular dynamics study of the gramicidin A channel in a DMPC bilayer. , 1996, 24, 92.		3
314	The calculation of the potential of mean force using computer simulations. Computer Physics Communications, 1995, 91, 275-282.	3.0	1,496
315	Potential energy function for cation-peptide interactions: Anab initio study. Journal of Computational Chemistry, 1995, 16, 690-704.	1.5	56
316	Numerical solution of the hypernetted chain equation for a solute of arbitrary geometry in three dimensions. Journal of Chemical Physics, 1995, 103, 360-364.	1.2	130
317	Conformational Flexibility of o-Phosphorylcholine and o-Phosphorylethanolamine: A Molecular Dynamics Study of Solvation Effects. Journal of the American Chemical Society, 1994, 116, 5916-5926.	6.6	117
318	Finite representation of an infinite bulk system: Solvent boundary potential for computer simulations. Journal of Chemical Physics, 1994, 100, 9050-9063.	1.2	911
319	Non-additivity in cationâ€”peptide interactions. A molecular dynamics and ab initio study of Na+ in the gramicidin channel. Chemical Physics Letters, 1993, 212, 231-240.	1.2	47
320	Ion transport in a gramicidin-like channel: dynamics and mobility. The Journal of Physical Chemistry, 1991, 95, 4856-4868.	2.9	171
321	The structure of gramicidin A in dimethylsulfoxide/acetone. FEBS Journal, 1990, 194, 57-60.	0.2	25
322	Solvation thermodynamics: An approach from analytic temperature derivatives. Journal of Chemical Physics, 1990, 92, 5020-5033.	1.2	132
323	Spatial dependence of timeâ€dependent friction for pair diffusion in a simple fluid. Journal of Chemical Physics, 1990, 93, 6804-6812.	1.2	66
324	Molecular basis for the Born model of ion solvation. The Journal of Physical Chemistry, 1990, 94, 4683-4688.	2.9	229

#	Article	IF	Citations
325	Engineering Dirhodium Artificial Metalloenzymes for Diazo Coupling Cascade Reactions**. Angewandte Chemie, 0, , .	1.6	0
326	Free Energy Methods in Drug Discoveryâ€”Introduction. ACS Symposium Series, 0, , 1-38.	0.5	24