Gregory A Voth

List of Publications by Year
in descending order

543 papers	42,572 citations	1994 101 h-index	4228 174 g-index
596 all docs	596 docs citations	596 times ranked	20844 citing authors

#	Article	IF	Citations
1	Key Factors Governing Initial Stages of Lipid Droplet Formation. Journal of Physical Chemistry B, 2022, 126, 453-462.	2.6	15
2	Using Machine Learning to Greatly Accelerate Path Integral <i>Ab Initio</i> Molecular Dynamics. Journal of Chemical Theory and Computation, 2022, 18, 599-604.	5.3	11
3	Multiscale Simulation of an Influenza A M2 Channel Mutant Reveals Key Features of Its Markedly Different Proton Transport Behavior. Journal of the American Chemical Society, 2022, 144, 769-776.	13.7	6
4	Ion permeation, selectivity, and electronic polarization in fluoride channels. Biophysical Journal, 2022, 121, 1336-1347.	0.5	12
5	Multiscale simulations of viruses. Biophysical Journal, 2022, 121, 330a.	0.5	0
6	Cooperative multivalent receptor binding promotes exposure of the SARS-CoV-2 fusion machinery core. Nature Communications, 2022, 13, 1002.	12.8	30
7	Strain and rupture of HIV-1 capsids during uncoating. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2117781119.	7.1	21
8	Computational Studies of Lipid Droplets. Journal of Physical Chemistry B, 2022, 126, 2145-2154.	2.6	19
9	Static and Dynamic Correlations in Water: Comparison of Classical Ab Initio Molecular Dynamics at Elevated Temperature with Path Integral Simulations at Ambient Temperature. Journal of Chemical Theory and Computation, 2022, 18, 2124-2131.	5.3	16
10	Seipin transmembrane segments critically function in triglyceride nucleation and lipid droplet budding from the membrane. ELife, 2022, 11, .	6.0	22
11	Proton coupling and the multiscale kinetic mechanism of a peptide transporter. Biophysical Journal, 2022, 121, 2266-2278.	0.5	9
12	Inositol Hexakisphosphate (IP6) Accelerates Immature HIV-1 Gag Protein Assembly toward Kinetically Trapped Morphologies. Journal of the American Chemical Society, 2022, 144, 10417-10428.	13.7	12
13	A multiscale coarse-grained model of the SARS-CoV-2 virion. Biophysical Journal, 2021, 120, 1097-1104.	0.5	139
14	Immature HIV-1 assembles from Gag dimers leaving partial hexamers at lattice edges as potential substrates for proteolytic maturation. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	40
15	Coarse-Grained Force Fields from the Perspective of Statistical Mechanics: Better Understanding of the Origins of a MARTINI Hangover. Journal of Chemical Theory and Computation, 2021, 17, 1170-1180.	5.3	46
16	Molecular interactions of theÂM and E integral membrane proteins of SARS-CoV-2. Faraday Discussions, 2021, 232, 49-67.	3.2	19
17	Structural basis of fast- and slow-severing actinâ€"cofilactin boundaries. Journal of Biological Chemistry, 2021, 296, 100337.	3.4	15
18	A new one-site coarse-grained model for water: Bottom-up many-body projected water (BUMPer). II. Temperature transferability and structural properties at low temperature. Journal of Chemical Physics, 2021, 154, 044105.	3.0	17

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19	Lipid-Composition-Mediated Forces Can Stabilize Tubular Assemblies of I-BAR Proteins. Biophysical Journal, 2021, 120, 46-54.	0.5	18
20	A new one-site coarse-grained model for water: Bottom-up many-body projected water (BUMPer). I. General theory and model. Journal of Chemical Physics, 2021, 154, 044104.	3.0	21
21	Constructing many-body dissipative particle dynamics models of fluids from bottom-up coarse-graining. Journal of Chemical Physics, 2021, 154, 084122.	3.0	23
22	Compressive and Tensile Deformations Alter ATP Hydrolysis and Phosphate Release Rates in Actin Filaments. Journal of Chemical Theory and Computation, 2021, 17, 1900-1913.	5.3	14
23	Modeling Protein-Lipid Interactions during Viral Assembly of SARS-CoV-2. Biophysical Journal, 2021, 120, 49a.	0.5	0
24	Synthesis, Characterization, and Simulation of Four-Armed Megamolecules. Biomacromolecules, 2021, 22, 2363-2372.	5.4	4
25	The hopping mechanism of the hydrated excess proton and its contribution to proton diffusion in water. Journal of Chemical Physics, 2021, 154, 194506.	3.0	12
26	Physical Characterization of Triolein and Implications for Its Role in Lipid Droplet Biogenesis. Journal of Physical Chemistry B, 2021, 125, 6874-6888.	2.6	13
27	Key computational findings reveal proton transfer as driving the functional cycle in the phosphate transporter PiPT. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	10
28	Structural Characterization of Protonated Water Clusters Confined in HZSM-5 Zeolites. Journal of the American Chemical Society, 2021, 143, 10203-10213.	13.7	35
29	Advanced Materials for Energy-Water Systems: The Central Role of Water/Solid Interfaces in Adsorption, Reactivity, and Transport. Chemical Reviews, 2021, 121, 9450-9501.	47.7	43
30	Formin Cdc12â€™s specific actin assembly properties are tailored for cytokinesis in fission yeast. Biophysical Journal, 2021, 120, 2984-2997.	0.5	6
31	Using Constrained Density Functional Theory to Track Proton Transfers and to Sample Their Associated Free Energy Surface. Journal of Chemical Theory and Computation, 2021, 17, 5759-5765.	5.3	9
32	Accurate and Transferable Reactive Molecular Dynamics Models from Constrained Density Functional Theory. Journal of Physical Chemistry B, 2021, 125, 10471-10480.	2.6	11
33	Integrin-based mechanosensing through conformational deformation. Biophysical Journal, 2021, 120, 4349-4359.	0.5	10
34	Resolving the Structural Debate for the Hydrated Excess Proton in Water. Journal of the American Chemical Society, 2021, 143, 18672-18683.	13.7	31
35	Preservation of HIV-1 Gag Helical Bundle Symmetry by Bevirimat Is Central to Maturation Inhibition. Journal of the American Chemical Society, 2021, 143, 19137-19148.	13.7	12
36	A quantitative paradigm for water-assisted proton transport through proteins and other confined spaces. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	16

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37	Local conformational dynamics regulating transport properties of a Cl â^' /H + antiporter. Journal of Computational Chemistry, 2020, 41, 513-519.	3.3	9
38	Temperature and Phase Transferable Bottom-up Coarse-Grained Models. Journal of Chemical Theory and Computation, 2020, 16, 6823-6842.	5.3	36
39	Molecular Origins of the Barriers to Proton Transport in Acidic Aqueous Solutions. Journal of Physical Chemistry B, 2020, 124, 8868-8876.	2.6	12
40	Multiscale Simulation Reveals Passive Proton Transport Through SERCA on the Microsecond Timescale. Biophysical Journal, 2020, 119, 1033-1040.	0.5	11
41	Structural basis for polarized elongation of actin filaments. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 30458-30464.	7.1	27
42	Minimal Experimental Bias on the Hydrogen Bond Greatly Improves Ab Initio Molecular Dynamics Simulations of Water. Journal of Chemical Theory and Computation, 2020, 16, 5675-5684.	5.3	9
43	Density Functional Theory-Based Quantum Mechanics/Coarse-Grained Molecular Mechanics: Theory and Implementation. Journal of Chemical Theory and Computation, 2020, 16, 6329-6342.	5.3	9
44	Atomic-scale characterization of mature HIV-1 capsid stabilization by inositol hexakisphosphate (IP) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	10.3	30
45	Influenza A M2 Inhibitor Binding Understood through Mechanisms of Excess Proton Stabilization and Channel Dynamics. Journal of the American Chemical Society, 2020, 142, 17425-17433.	13.7	19
46	Microtubule Simulations Provide Insight into the Molecular Mechanism Underlying Dynamic Instability. Biophysical Journal, 2020, 118, 2938-2951.	0.5	22
47	A helical assembly of human ESCRT-I scaffolds reverse-topology membrane scission. Nature Structural and Molecular Biology, 2020, 27, 570-580.	8.2	44
48	What Coordinate Best Describes the Affinity of the Hydrated Excess Proton for the Airâ€"Water Interface?. Journal of Physical Chemistry B, 2020, 124, 5039-5046.	2.6	9
49	Interfacial solvation and slow transport of hydrated excess protons in non-ionic reverse micelles. Physical Chemistry Chemical Physics, 2020, 22, 10753-10763.	2.8	4
50	TRIM5Î± self-assembly and compartmentalization of the HIV-1 viral capsid. Nature Communications, 2020, 11, 1307.	12.8	51
51	Water-Assisted Proton Transport in Confined Nanochannels. Journal of Physical Chemistry C, 2020, 124, 16186-16201.	3.1	12
52	Cholesterol Alters the Orientation and Activity of the Influenza Virus M2 Amphipathic Helix in the Membrane. Journal of Physical Chemistry B, 2020, 124, 6738-6747.	2.6	22
53	Reactive Coarse-Grained Molecular Dynamics. Journal of Chemical Theory and Computation, 2020, 16, 2541-2549.	5.3	11
54	Modeling Synthesized Protein Megamolecules: Structure, Dynamics, and Functions. Biophysical Journal, 2020, 118, 517a.	0.5	0

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55	Anisotropic Motions of Fibrils Dictated by Their Orientations in the Lamella: A Coarse-Grained Model of a Plant Cell Wall. Journal of Physical Chemistry B, 2020, 124, 3527-3539.	2.6	9
56	Binding mechanism of the matrix domain of HIV-1 gag on lipid membranes. ELife, 2020, 9, .	6.0	21
57	Dynamic Protonation Dramatically Affects the Membrane Permeability of Drug-like Molecules. Journal of the American Chemical Society, 2019, 141, 13421-13433.	13.7	56
58	Plastic Deformation and Fragmentation of Strained Actin Filaments. Biophysical Journal, 2019, 117, 453-463.	0.5	19
59	Understanding Missing Entropy in Coarse-Grained Systems: Addressing Issues of Representability and Transferability. Journal of Physical Chemistry Letters, 2019, 10, 4549-4557.	4.6	51
60	Mechanical and kinetic factors drive sorting of F-actin cross-linkers on bundles. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 16192-16197.	7.1	43
61	Unusual Organization of I-BAR Proteins on Tubular and Vesicular Membranes. Biophysical Journal, 2019, 117, 553-562.	0.5	27
62	Proton-Induced Conformational and Hydration Dynamics in the Influenza A M2 Channel. Journal of the American Chemical Society, 2019, 141, 11667-11676.	13.7	28
63	Compatible observable decompositions for coarse-grained representations of real molecular systems. Journal of Chemical Physics, 2019, 151, 134115.	3.0	16
64	Adversarial-residual-coarse-graining: Applying machine learning theory to systematic molecular coarse-graining. Journal of Chemical Physics, 2019, 151, 124110.	3.0	30
65	Systematic Coarse-Grained Lipid Force Fields with Semiexplicit Solvation via Virtual Sites. Journal of Chemical Theory and Computation, 2019, 15, 2087-2100.	5.3	26
66	Coarse-graining of many-body path integrals: Theory and numerical approximations. Journal of Chemical Physics, 2019, 150, 244103.	3.0	2
67	Off-Pathway Assembly: A Broad-Spectrum Mechanism of Action for Drugs That Undermine Controlled HIV-1 Viral Capsid Formation. Journal of the American Chemical Society, 2019, 141, 10214-10224.	13.7	38
68	Multiscale model of integrin adhesion assembly. PLoS Computational Biology, 2019, 15, e1007077.	3.2	34
69	Coarse-graining involving virtual sites: Centers of symmetry coarse-graining. Journal of Chemical Physics, 2019, 150, 154103.	3.0	16
70	Multiconfigurational Coarse-Grained Molecular Dynamics. Journal of Chemical Theory and Computation, 2019, 15, 3306-3315.	5.3	22
71	Coarse-Grained Simulation of Full-Length Integrin Activation. Biophysical Journal, 2019, 116, 1000-1010.	0.5	22
72	Ena/VASP processive elongation is modulated by avidity on actin filaments bundled by the filopodia cross-linker fascin. Molecular Biology of the Cell, 2019, 30, 851-862.	2.1	44

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73	Lamellipodium is a myosin-independent mechanosensor. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 2646-2651.	7.1	101
74	Quantum mechanics/coarse-grained molecular mechanics (QM/CG-MM). Journal of Chemical Physics, 2018, 148, 014102.	3.0	11
75	Multiscale Kinetic Modeling Reveals an Ensemble of Cl^{â€“}/H⁺ Exchange Pathways in ClC-ec1 Antiporter. Journal of the American Chemical Society, 2018, 140, 1793-1804.	13.7	39
76	Quantum theory of multiscale coarse-graining. Journal of Chemical Physics, 2018, 148, 102335.	3.0	13
77	Mechanism and Determinants of Amphipathic Helix-Containing Protein Targeting to Lipid Droplets. Developmental Cell, 2018, 44, 73-86.e4.	7.0	175
78	Organizing membrane-curving proteins: the emerging dynamical picture. Current Opinion in Structural Biology, 2018, 51, 99-105.	5.7	34
79	Ultra-Coarse-Grained Models Allow for an Accurate and Transferable Treatment of Interfacial Systems. Journal of Chemical Theory and Computation, 2018, 14, 2180-2197.	5.3	52
80	Modulating the Chemical Transport Properties of a Transmembrane Antiporter via Alternative Anion Flux. Journal of the American Chemical Society, 2018, 140, 16535-16543.	13.7	24
81	Editorial overview: COSB biophysical and computational methods. Current Opinion in Structural Biology, 2018, 52, vi-vii.	5.7	0
82	Advances in coarse-grained modeling of macromolecular complexes. Current Opinion in Structural Biology, 2018, 52, 119-126.	5.7	100
83	Ultra-Coarse-Grained Liquid State Models with Implicit Hydrogen Bonding. Journal of Chemical Theory and Computation, 2018, 14, 6159-6174.	5.3	22
84	Multiscale simulation of actin filaments and actin-associated proteins. Biophysical Reviews, 2018, 10, 1521-1535.	3.2	7
85	Insights into the Cooperative Nature of ATP Hydrolysis in Actin Filaments. Biophysical Journal, 2018, 115, 1589-1602.	0.5	29
86	Mesoscopic coarse-grained representations of fluids rigorously derived from atomistic models. Journal of Chemical Physics, 2018, 149, 044104.	3.0	23
87	The 2018 biomembrane curvature and remodeling roadmap. Journal Physics D: Applied Physics, 2018, 51, 343001.	2.8	212
88	Entropic forces drive clustering and spatial localization of influenza A M2 during viral budding. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E8595-E8603.	7.1	47
89	Molecular transport through membranes: Accurate permeability coefficients from multidimensional potentials of mean force and local diffusion constants. Journal of Chemical Physics, 2018, 149, 072310.	3.0	43
90	Gating mechanisms during actin filament elongation by formins. ELife, 2018, 7, .	6.0	25

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91	Simulations of N-BAR Protein Interactions with Membranes. Journal Physics D: Applied Physics, 2018, 51, 35-36.	2.8	0
92	The Theory of Ultra-Coarse-Graining. 3. Coarse-Grained Sites with Rapid Local Equilibrium of Internal States. Journal of Chemical Theory and Computation, 2017, 13, 1010-1022.	5.3	54
93	Highly Coarse-Grained Representations of Transmembrane Proteins. Journal of Chemical Theory and Computation, 2017, 13, 935-944.	5.3	17
94	Communication: Improved <i>ab initio</i> molecular dynamics by minimally biasing with experimental data. Journal of Chemical Physics, 2017, 146, 041102.	3.0	20
95	IR spectral assignments for the hydrated excess proton in liquid water. Journal of Chemical Physics, 2017, 146, 154507.	3.0	61
96	Reactive molecular dynamics models from ab initio molecular dynamics data using relative entropy minimization. Chemical Physics Letters, 2017, 683, 573-578.	2.6	4
97	Non-uniqueness of quantum transition state theory and general dividing surfaces in the path integral space. Journal of Chemical Physics, 2017, 146, 174106.	3.0	5
98	Friction Mediates Scission of Tubular Membranes Scaffolded by BAR Proteins. Cell, 2017, 170, 172-184.e11.	28.9	171
99	Role of solvation structure in the shuttling of the hydrated excess proton. Journal of Chemical Sciences, 2017, 129, 1045-1051.	1.5	4
100	Understanding the essential proton-pumping kinetic gates and decoupling mutations in cytochrome <i>c</i> oxidase. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 5924-5929.	7.1	40
101	The Origin of Coupled Chloride and Proton Transport in a Cl - /H + Antiporter. Biophysical Journal, 2017, 112, 254a-255a.	0.5	0
102	Simulating Protein Mediated Hydrolysis of ATP and Other Nucleoside Triphosphates by Combining QM/MM Molecular Dynamics with Advances in Metadynamics. Journal of Chemical Theory and Computation, 2017, 13, 2332-2341.	5.3	40
103	A Multiscale Description of Biomolecular Active Matter: The Chemistry Underlying Many Life Processes. Accounts of Chemical Research, 2017, 50, 594-598.	15.6	18
104	Mechanoregulated inhibition of formin facilitates contractile actomyosin ring assembly. Nature Communications, 2017, 8, 703.	12.8	66
105	Phosphomimetic S3D cofilin binds but only weakly severs actin filaments. Journal of Biological Chemistry, 2017, 292, 19565-19579.	3.4	35
106	Delocalization and stretch-bend mixing of the HOH bend in liquid water. Journal of Chemical Physics, 2017, 147, 084503.	3.0	51
107	The mesoscopic membrane with proteins (MesM-P) model. Journal of Chemical Physics, 2017, 147, 044101.	3.0	20
108	Actin Filament Strain Promotes Severing and Cofilin Dissociation. Biophysical Journal, 2017, 112, 2624-2633.	0.5	49

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109	Extending the range and physical accuracy of coarse-grained models: Order parameter dependent interactions. Journal of Chemical Physics, 2017, 147, 044113.	3.0	53
110	Coarse-Grained Directed Simulation. Journal of Chemical Theory and Computation, 2017, 13, 4593-4603.	5.3	11
111	Development of reactive force fields using <i>ab initio</i> molecular dynamics simulation minimally biased to experimental data. Journal of Chemical Physics, 2017, 147, 161719.	3.0	12
112	Long-Range Organization of Membrane-Curving Proteins. ACS Central Science, 2017, 3, 1246-1253.	11.3	36
113	Proton movement and coupling in the POT family of peptide transporters. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 13182-13187.	7.1	81
114	Immature HIV-1 lattice assembly dynamics are regulated by scaffolding from nucleic acid and the plasma membrane. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E10056-E10065.	7.1	86
115	Competition between Tropomyosin, Fimbrin, and ADF/Cofilin drives their sorting to distinct actin filament networks. ELife, 2017, 6, .	6.0	76
116	Molecular modeling and assignment of IR spectra of the hydrated excess proton in isotopically dilute water. Journal of Chemical Physics, 2016, 145, 154504.	3.0	19
117	Dynamic force matching: Construction of dynamic coarse-grained models with realistic short time dynamics and accurate long time dynamics. Journal of Chemical Physics, 2016, 145, 224107.	3.0	33
118	Can quantum transition state theory be defined as an exact <i>t</i> = 0+ limit?. Journal of Chemical Physics, 2016, 144, 084110.	3.0	7
119	On the representability problem and the physical meaning of coarse-grained models. Journal of Chemical Physics, 2016, 145, 044108.	3.0	103
120	Multiscale Simulations Reveal Key Aspects of the Proton Transport Mechanism in the ClC-ec1 Antiporter. Biophysical Journal, 2016, 110, 1334-1345.	0.5	55
121	Coupling Protein Dynamics with Proton Transport in Human Carbonic Anhydrase II. Journal of Physical Chemistry B, 2016, 120, 8389-8404.	2.6	27
122	A Direct Method for Incorporating Experimental Data into Multiscale Coarse-Grained Models. Journal of Chemical Theory and Computation, 2016, 12, 2144-2153.	5.3	29
123	Transition-Tempered Metadynamics Is a Promising Tool for Studying the Permeation of Drug-like Molecules through Membranes. Journal of Chemical Theory and Computation, 2016, 12, 5157-5169.	5.3	54
124	Fascin- and Î±-Actinin-Bundled Networks Contain Intrinsic Structural Features that Drive Protein Sorting. Current Biology, 2016, 26, 2697-2706.	3.9	104
125	How curvature-generating proteins build scaffolds on membrane nanotubes. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 11226-11231.	7.1	120
126	Acid activation mechanism of the influenza A M2 proton channel. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E6955-E6964.	7.1	81

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127	The Origin of Coupled Chloride and Proton Transport in a Cl^{â€“}/H⁺ Antiporter. Journal of the American Chemical Society, 2016, 138, 14923-14930.	13.7	41
128	Coarse-grained simulation reveals key features of HIV-1 capsid self-assembly. Nature Communications, 2016, 7, 11568.	12.8	134
129	Multiscale simulations reveal key features of the proton-pumping mechanism in cytochrome <i>c</i> oxidase. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 7420-7425.	7.1	60
130	Multiscale simulations of protein-facilitated membrane remodeling. Journal of Structural Biology, 2016, 196, 57-63.	2.8	14
131	Selective Targeting of Lipid Droplets by Proteins. Biophysical Journal, 2016, 110, 574a.	0.5	0
132	The F-actin bundler Î±-actinin Ain1 is tailored for ring assembly and constriction during cytokinesis in fission yeast. Molecular Biology of the Cell, 2016, 27, 1821-1833.	2.1	47
133	Role of Presolvation and Anharmonicity in Aqueous Phase Hydrated Proton Solvation and Transport. Journal of Physical Chemistry B, 2016, 120, 1793-1804.	2.6	68
134	Cations Stiffen Actin Filaments by Adhering a Key Structural Element to Adjacent Subunits. Journal of Physical Chemistry B, 2016, 120, 4558-4567.	2.6	39
135	Hydroxide Solvation and Transport in Anion Exchange Membranes. Journal of the American Chemical Society, 2016, 138, 991-1000.	13.7	208
136	Proton Solvation and Transport in Realistic Proton Exchange Membrane Morphologies. Journal of Physical Chemistry C, 2016, 120, 3176-3186.	3.1	39
137	Computationally Efficient Multiscale Reactive Molecular Dynamics to Describe Amino Acid Deprotonation in Proteins. Journal of Chemical Theory and Computation, 2016, 12, 879-891.	5.3	52
138	A reductionist perspective on quantum statistical mechanics: Coarse-graining of path integrals. Journal of Chemical Physics, 2015, 143, 094104.	3.0	9
139	The multiscale coarse-graining method. XI. Accurate interactions based on the centers of charge of coarse-grained sites. Journal of Chemical Physics, 2015, 143, 243116.	3.0	31
140	Membrane tension controls the assembly of curvature-generating proteins. Nature Communications, 2015, 6, 7219.	12.8	141
141	Mesoscale Study of Proton Transport in Proton Exchange Membranes: Role of Morphology. Journal of Physical Chemistry C, 2015, 119, 1753-1762.	3.1	30
142	Ion Transport through Ultrathin Electrolyte under Applied Voltages. Journal of Physical Chemistry B, 2015, 119, 7516-7521.	2.6	12
143	Hydrated Excess Protons Can Create Their Own Water Wires. Journal of Physical Chemistry B, 2015, 119, 9212-9218.	2.6	83
144	Electrostatic Interactions between the Bni1p Formin FH2 Domain and Actin Influence Actin Filament Nucleation. Structure, 2015, 23, 68-79.	3.3	24

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145	An analysis of hydrated proton diffusion in <i>ab initio</i> molecular dynamics. Journal of Chemical Physics, 2015, 142, 014104.	3.0	63
146	Hydrated Proton Structure and Diffusion at Platinum Surfaces. Journal of Physical Chemistry C, 2015, 119, 14675-14682.	3.1	13
147	Predicting the Sensitivity of Multiscale Coarse-Grained Models to their Underlying Fine-Grained Model Parameters. Journal of Chemical Theory and Computation, 2015, 11, 3547-3560.	5.3	13
148	Designing Free Energy Surfaces That Match Experimental Data with Metadynamics. Journal of Chemical Theory and Computation, 2015, 11, 2451-2460.	5.3	49
149	Propensity of Hydrated Excess Protons and Hydroxide Anions for the Airâ€"Water Interface. Journal of the American Chemical Society, 2015, 137, 12610-12616.	13.7	100
150	When Physics Takes Over: BAR Proteins and Membrane Curvature. Trends in Cell Biology, 2015, 25, 780-792.	7.9	247
151	Exploring Valleys without Climbing Every Peak: More Efficient and Forgiving Metabasin Metadynamics via Robust On-the-Fly Bias Domain Restriction. Journal of Chemical Theory and Computation, 2015, 11, 5638-5650.	5.3	31
152	Dynamic force matching: A method for constructing dynamical coarse-grained models with realistic time dependence. Journal of Chemical Physics, 2015, 142, 154104.	3.0	86
153	Ion mixing, hydration, and transport in aqueous ionic systems. Journal of Chemical Physics, 2015, 142, 184905.	3.0	13
154	Electron transfer activation of a second water channel for proton transport in [FeFe]-hydrogenase. Journal of Chemical Physics, 2014, 141, 22D527.	3.0	21
155	Solvent-Free, Highly Coarse-Grained Models for Charged Lipid Systems. Journal of Chemical Theory and Computation, 2014, 10, 4730-4744.	5.3	20
156	Can the ring polymer molecular dynamics method be interpreted as real time quantum dynamics?. Journal of Chemical Physics, 2014, 140, 154103.	3.0	26
157	The Theory of Ultra-Coarse-Graining. 2. Numerical Implementation. Journal of Chemical Theory and Computation, 2014, 10, 5265-5275.	5.3	60
158	Highly Scalable and Memory Efficient Ultra-Coarse-Grained Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2014, 10, 423-431.	5.3	26
159	Persistent Subdiffusive Proton Transport in Perfluorosulfonic Acid Membranes. Journal of Physical Chemistry Letters, 2014, 5, 3037-3042.	4.6	33
160	Special Issue on Free Energy. Journal of Chemical Theory and Computation, 2014, 10, 2631-2631.	5.3	5
161	Well-Tempered Metadynamics Converges Asymptotically. Physical Review Letters, 2014, 112, 240602.	7.8	248
162	Proton Transport under External Applied Voltage. Journal of Physical Chemistry B, 2014, 118, 8090-8098.	2.6	19

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163	Interactions of Protein Kinase C-Î± C1A and C1B Domains with Membranes: A Combined Computational and Experimental Study. Journal of the American Chemical Society, 2014, 136, 11757-11766.	13.7	31
164	Benchmark Study of the SCC-DFTB Approach for a Biomolecular Proton Channel. Journal of Chemical Theory and Computation, 2014, 10, 451-462.	5.3	31
165	Chloride Enhances Fluoride Mobility in Anion Exchange Membrane/Polycationic Systems. Journal of Physical Chemistry C, 2014, 118, 845-853.	3.1	24
166	Insights into the Transport of Aqueous Quaternary Ammonium Cations: A Combined Experimental and Computational Study. Journal of Physical Chemistry B, 2014, 118, 1363-1372.	2.6	22
167	Unraveling the Mystery of ATP Hydrolysis in Actin Filaments. Journal of the American Chemical Society, 2014, 136, 13053-13058.	13.7	74
168	Transition-Tempered Metadynamics: Robust, Convergent Metadynamics via On-the-Fly Transition Barrier Estimation. Journal of Chemical Theory and Computation, 2014, 10, 3626-3633.	5.3	70
169	Nucleotide Regulation of the Structure and Dynamics of G-Actin. Biophysical Journal, 2014, 106, 1710-1720.	0.5	22
170	Path Integral Coarse-Graining Replica Exchange Method for Enhanced Sampling. Journal of Chemical Theory and Computation, 2014, 10, 3634-3640.	5.3	11
171	Efficient and Minimal Method to Bias Molecular Simulations with Experimental Data. Journal of Chemical Theory and Computation, 2014, 10, 3023-3030.	5.3	90
172	Proton Transport Mechanism of Perfluorosulfonic Acid Membranes. Journal of Physical Chemistry C, 2014, 118, 17436-17445.	3.1	84
173	Multiscale simulation reveals a multifaceted mechanism of proton permeation through the influenza A M2 proton channel. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 9396-9401.	7.1	81
174	Nucleotide-Dependent Lateral and Longitudinal Interactions in Microtubules. Journal of Molecular Biology, 2013, 425, 2232-2246.	4.2	32
175	Molecular Mechanism of Membrane Binding of the GRP1 PH Domain. Journal of Molecular Biology, 2013, 425, 3073-3090.	4.2	56
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