Gregory A Voth

List of Publications by Year
in descending order

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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	A Multiscale Coarse-Graining Method for Biomolecular Systems. Journal of Physical Chemistry B, 2005, 109, 2469-2473.	2.6	1,018
2	Flexible simple point-charge water model with improved liquid-state properties. Journal of Chemical Physics, 2006, 124, 024503.	3.0	955
3	Unique Spatial Heterogeneity in Ionic Liquids. Journal of the American Chemical Society, 2005, 127, 12192-12193.	13.7	919
4	The multiscale coarse-graining method. I. A rigorous bridge between atomistic and coarse-grained models. Journal of Chemical Physics, 2008, 128, 244114.	3.0	651
5	On the Structure and Dynamics of Ionic Liquids. Journal of Physical Chemistry B, 2004, 108, 1744-1752.	2.6	649
6	The computer simulation of proton transport in water. Journal of Chemical Physics, 1999, 111, 9361-9381.	3.0	557
7	Multiscale coarse graining of liquid-state systems. Journal of Chemical Physics, 2005, 123, 134105.	3.0	531
8	Rigorous formulation of quantum transition state theory and its dynamical corrections. Journal of Chemical Physics, 1989, 91, 7749-7760.	3.0	498
9	Coarse-Graining Methods for Computational Biology. Annual Review of Biophysics, 2013, 42, 73-93.	10.0	475
10	The formulation of quantum statistical mechanics based on the Feynman path centroid density. II. Dynamical properties. Journal of Chemical Physics, 1994, 100, 5106-5117.	3.0	454
11	Molecular Dynamics Simulation of Nanostructural Organization in Ionic Liquid/Water Mixturesâ€. Journal of Physical Chemistry B, 2007, 111, 4812-4818.	2.6	431
12	Ab initio molecular dynamics: Propagating the density matrix with Gaussian orbitals. III. Comparison with Bornâ€“Oppenheimer dynamics. Journal of Chemical Physics, 2002, 117, 8694-8704.	3.0	430
13	Multistate Empirical Valence Bond Model for Proton Transport in Water. Journal of Physical Chemistry B, 1998, 102, 5547-5551.	2.6	397
14	Computer Simulation of Proton Solvation and Transport in Aqueous and Biomolecular Systems. Accounts of Chemical Research, 2006, 39, 143-150.	15.6	395
15	Multiscale modeling of biomolecular systems: in serial and in parallel. Current Opinion in Structural Biology, 2007, 17, 192-198.	5.7	395
16	Molecular Dynamics Simulation of Ionic Liquids:â€‰ The Effect of Electronic Polarizability. Journal of Physical Chemistry B, 2004, 108, 11877-11881.	2.6	393
17	Tail Aggregation and Domain Diffusion in Ionic Liquids. Journal of Physical Chemistry B, 2006, 110, 18601-18608.	2.6	387
18	Effective force fields for condensed phase systems from ab initio molecular dynamics simulation: A new method for force-matching. Journal of Chemical Physics, 2004, 120, 10896-10913.	3.0	383

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19	Ab initio molecular dynamics: Propagating the density matrix with Gaussian orbitals. II. Generalizations based on mass-weighting, idempotency, energy conservation and choice of initial conditions. Journal of Chemical Physics, 2001, 115, 10291.	3.0	375
20	The quantum dynamics of an excess proton in water. Journal of Chemical Physics, 1996, 104, 2056-2069.	3.0	328
21	The multiscale coarse-graining method. II. Numerical implementation for coarse-grained molecular models. Journal of Chemical Physics, 2008, 128, 244115.	3.0	326
22	Understanding Ionic Liquids through Atomistic and Coarse-Grained Molecular Dynamics Simulations. Accounts of Chemical Research, 2007, 40, 1193-1199.	15.6	304
23	The formulation of quantum statistical mechanics based on the Feynman path centroid density. IV. Algorithms for centroid molecular dynamics. Journal of Chemical Physics, 1994, 101, 6168-6183.	3.0	299
24	The formulation of quantum statistical mechanics based on the Feynman path centroid density. I. Equilibrium properties. Journal of Chemical Physics, 1994, 100, 5093-5105.	3.0	298
25	Special Pair Dance and Partner Selection: Elementary Steps in Proton Transport in Liquid Water. Journal of Physical Chemistry B, 2008, 112, 9456-9466.	2.6	291
26	A second generation multistate empirical valence bond model for proton transport in aqueous systems. Journal of Chemical Physics, 2002, 117, 5839-5849.	3.0	285
27	Proton Solvation and Transport in Aqueous and Biomolecular Systems:Â Insights from Computer Simulations. Journal of Physical Chemistry B, 2007, 111, 4300-4314.	2.6	279
28	The Curious Case of the Hydrated Proton. Accounts of Chemical Research, 2012, 45, 101-109.	15.6	266
29	A derivation of centroid molecular dynamics and other approximate time evolution methods for path integral centroid variables. Journal of Chemical Physics, 1999, 111, 2371-2384.	3.0	261
30	Ionic Liquids. Accounts of Chemical Research, 2007, 40, 1077-1078.	15.6	259
31	The Hydrated Proton at the Water Liquid/Vapor Interface. Journal of Physical Chemistry B, 2004, 108, 14804-14806.	2.6	255
32	Well-Tempered Metadynamics Converges Asymptotically. Physical Review Letters, 2014, 112, 240602.	7.8	248
33	When Physics Takes Over: BAR Proteins and Membrane Curvature. Trends in Cell Biology, 2015, 25, 780-792.	7.9	247
34	Further developments in the local-orbital density-functional-theory tight-binding method. Physical Review B, 2001, 64, .	3.2	232
35	Mixed Atomistic and Coarse-Grained Molecular Dynamics:Â Simulation of a Membrane-Bound Ion Channel. Journal of Physical Chemistry B, 2006, 110, 15045-15048.	2.6	230
36	A bond-order analysis of the mechanism for hydrated proton mobility in liquid water. Journal of Chemical Physics, 2005, 122, 014506.	3.0	229

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37	An Improved Multistate Empirical Valence Bond Model for Aqueous Proton Solvation and Transport. Journal of Physical Chemistry B, 2008, 112, 467-482.	2.6	228
38	The formulation of quantum statistical mechanics based on the Feynman path centroid density. III. Phase space formalism and analysis of centroid molecular dynamics. Journal of Chemical Physics, 1994, 101, 6157-6167.	3.0	225
39	A new perspective on quantum time correlation functions. Journal of Chemical Physics, 1993, 99, 10070-10073.	3.0	224
40	Structural Basis of Membrane Bending by the N-BAR Protein Endophilin. Cell, 2012, 149, 137-145.	28.9	220
41	Direct observation of Bin/amphiphysin/Rvs (BAR) domain-induced membrane curvature by means of molecular dynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 15068-15072.	7.1	218
42	The 2018 biomembrane curvature and remodeling roadmap. Journal Physics D: Applied Physics, 2018, 51, 343001.	2.8	212
43	Hydroxide Solvation and Transport in Anion Exchange Membranes. Journal of the American Chemical Society, 2016, 138, 991-1000.	13.7	208
44	The vibrational spectrum of the hydrated proton: Comparison of experiment, simulation, and normal mode analysis. Journal of Chemical Physics, 2002, 116, 737-746.	3.0	200
45	The Properties of Water: Insights from Quantum Simulations. Journal of Physical Chemistry B, 2009, 113, 5702-5719.	2.6	199
46	Structure of the Liquidâ^'Vacuum Interface of Room-Temperature Ionic Liquids:Â A Molecular Dynamics Study. Journal of Physical Chemistry B, 2006, 110, 1800-1806.	2.6	195
47	Multiscale Coarse-Graining and Structural Correlations:Â Connections to Liquid-State Theory. Journal of Physical Chemistry B, 2007, 111, 4116-4127.	2.6	191
48	Path integral centroid variables and the formulation of their exact real time dynamics. Journal of Chemical Physics, 1999, 111, 2357-2370.	3.0	190
49	A quantum model for water: Equilibrium and dynamical properties. Journal of Chemical Physics, 1997, 106, 2400-2410.	3.0	187
50	An accurate and simple quantum model for liquid water. Journal of Chemical Physics, 2006, 125, 184507.	3.0	187
51	Modeling real dynamics in the coarse-grained representation of condensed phase systems. Journal of Chemical Physics, 2006, 125, 151101.	3.0	184
52	Mechanism of Membrane Curvature Sensing by Amphipathic Helix Containing Proteins. Biophysical Journal, 2011, 100, 1271-1279.	0.5	184
53	Molecular dynamics simulations of imidazolium-based ionic liquid/water mixtures: Alkyl side chain length and anion effects. Fluid Phase Equilibria, 2010, 294, 148-156.	2.5	182
54	The Mechanism of Hydrated Proton Transport in Water. Journal of the American Chemical Society, 2000, 122, 12027-12028.	13.7	180

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55	The Formation and Dynamics of Proton Wires in Channel Environments. Biophysical Journal, 2001, 80, 1691-1702.	0.5	178
56	Allostery of actin filaments: Molecular dynamics simulations and coarse-grained analysis. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 13111-13116.	7.1	178
57	Coarse-Grained Modeling of the Actin Filament Derived from Atomistic-Scale Simulations. Biophysical Journal, 2006, 90, 1572-1582.	0.5	178
58	Coarse-Grained Peptide Modeling Using a Systematic Multiscale Approach. Biophysical Journal, 2007, 92, 4289-4303.	0.5	176
59	Mechanism and Determinants of Amphipathic Helix-Containing Protein Targeting to Lipid Droplets. Developmental Cell, 2018, 44, 73-86.e4.	7.0	175
60	Transition State Dynamics and Relaxation Processes in Solutions:Â A Frontier of Physical Chemistry. The Journal of Physical Chemistry, 1996, 100, 13034-13049.	2.9	174
61	Multiscale Coarse-Graining of Ionic Liquidsâ€. Journal of Physical Chemistry B, 2006, 110, 3564-3575.	2.6	174
62	Characterization of the Solvation and Transport of the Hydrated Proton in the Perfluorosulfonic Acid Membrane Nafion. Journal of Physical Chemistry B, 2006, 110, 18594-18600.	2.6	171
63	Friction Mediates Scission of Tubular Membranes Scaffolded by BAR Proteins. Cell, 2017, 170, 172-184.e11.	28.9	171
64	A Systematic Methodology for Defining Coarse-Grained Sites in Large Biomolecules. Biophysical Journal, 2008, 95, 5073-5083.	0.5	153
65	The Theory of Electron Transfer Reactions:Â What May Be Missing?. Journal of the American Chemical Society, 2003, 125, 7470-7478.	13.7	152
66	Quantum effects in liquid water from an ab initio-based polarizable force field. Journal of Chemical Physics, 2007, 127, 074506.	3.0	151
67	The Theory of Ultra-Coarse-Graining. 1. General Principles. Journal of Chemical Theory and Computation, 2013, 9, 2466-2480.	5.3	149
68	The mechanism of proton exclusion in aquaporin channels. Proteins: Structure, Function and Bioinformatics, 2004, 55, 223-228.	2.6	148
69	Systematic Multiscale Parameterization of Heterogeneous Elastic Network Models of Proteins. Biophysical Journal, 2008, 95, 4183-4192.	0.5	148
70	Path-Integral Centroid Methods in Quantum Statistical Mechanics and Dynamics. Advances in Chemical Physics, 2007, , 135-218.	0.3	145
71	Mechanism of Fast Proton Transport along One-Dimensional Water Chains Confined in Carbon Nanotubes. Journal of the American Chemical Society, 2010, 132, 11395-11397.	13.7	144
72	Linear aggregation of proteins on the membrane as a prelude to membrane remodeling. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 20396-20401.	7.1	144

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73	Proton Transfer in the Enzyme Carbonic Anhydrase:Â Anab InitioStudy. Journal of the American Chemical Society, 1998, 120, 4006-4014.	13.7	143
74	Membrane tension controls the assembly of curvature-generating proteins. Nature Communications, 2015, 6, 7219.	12.8	141
75	A multiscale coarse-grained model of the SARS-CoV-2 virion. Biophysical Journal, 2021, 120, 1097-1104.	0.5	139
76	Multiscale Coarse-Graining of Mixed Phospholipid/Cholesterol Bilayers. Journal of Chemical Theory and Computation, 2006, 2, 637-648.	5.3	138
77	Atomistic Modeling of the Electrodeâ€“Electrolyte Interface in Li-Ion Energy Storage Systems: Electrolyte Structuring. Journal of Physical Chemistry C, 2013, 117, 3747-3761.	3.1	137
78	Coarse-grained simulation reveals key features of HIV-1 capsid self-assembly. Nature Communications, 2016, 7, 11568.	12.8	134
79	Hybrid Ab-Initio/Empirical Molecular Dynamics:â€‰ Combining the ONIOM Scheme with the Atom-Centered Density Matrix Propagation (ADMP) Approach. Journal of Physical Chemistry B, 2004, 108, 4210-4220.	2.6	131
80	A comparative study of imaginary time path integral based methods for quantum dynamics. Journal of Chemical Physics, 2006, 124, 154103.	3.0	131
81	Exact exchange in ab initio molecular dynamics: An efficient plane-wave based algorithm. Journal of Chemical Physics, 1998, 108, 4697-4700.	3.0	130
82	Probing Selected Morphological Models of Hydrated Nafion Using Large-Scale Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2010, 114, 3205-3218.	2.6	129
83	Proton Solvation and Transport in Hydrated Nafion. Journal of Physical Chemistry B, 2011, 115, 5903-5912.	2.6	125
84	Coarse-Grained Free Energy Functions for Studying Protein Conformational Changes: A Double-Well Network Model. Biophysical Journal, 2007, 93, 3860-3871.	0.5	124
85	Effective force coarse-graining. Physical Chemistry Chemical Physics, 2009, 11, 2002.	2.8	124
86	Infrared Spectroscopy and Hydrogen-Bond Dynamics of Liquid Water from Centroid Molecular Dynamics with an Ab Initio-Based Force Field. Journal of Physical Chemistry B, 2009, 113, 13118-13130.	2.6	123
87	Excess Proton Solvation and Delocalization in a Hydrophilic Pocket of the Proton Conducting Polymer Membrane Nafion. Journal of Physical Chemistry B, 2005, 109, 3727-3730.	2.6	122
88	Applications of higher order composite factorization schemes in imaginary time path integral simulations. Journal of Chemical Physics, 2001, 115, 7832-7842.	3.0	120
89	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
90	The formulation of quantum statistical mechanics based on the Feynman path centroid density. V. Quantum instantaneous normal mode theory of liquids. Journal of Chemical Physics, 1994, 101, 6184-6192.	3.0	118

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91	A Role for a Specific Cholesterol Interaction in Stabilizing the Apo Configuration of the Human A 2A Adenosine Receptor. Structure, 2009, 17, 1660-1668.	3.3	118
92	Multiscale Coarse-Graining of the Protein Energy Landscape. PLoS Computational Biology, 2010, 6, e1000827.	3.2	116
93	Charge Delocalization in Proton Channels, I: The Aquaporin Channels and Proton Blockage. Biophysical Journal, 2007, 92, 46-60.	0.5	114
94	The multiscale coarse-graining method. VI. Implementation of three-body coarse-grained potentials. Journal of Chemical Physics, 2010, 132, 164107.	3.0	113
95	Calculation of solvent free energies for heterogeneous electron transfer at the waterâ€“metal interface: Classical versus quantum behavior. Journal of Chemical Physics, 1995, 102, 529-539.	3.0	112
96	Molecular Dynamics Simulation of Proton Transport through the Influenza A Virus M2 Channel. Biophysical Journal, 2002, 83, 1987-1996.	0.5	111
97	Efficient, Regularized, and Scalable Algorithms for Multiscale Coarse-Graining. Journal of Chemical Theory and Computation, 2010, 6, 954-965.	5.3	110
98	Systematic Coarse-Graining of Nanoparticle Interactions in Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2005, 109, 17019-17024.	2.6	109
99	The multiscale coarse-graining method. IV. Transferring coarse-grained potentials between temperatures. Journal of Chemical Physics, 2009, 131, 024103.	3.0	108
100	Carâ€“Parrinello molecular dynamics simulation of liquid water: New results. Journal of Chemical Physics, 2002, 116, 10372-10376.	3.0	106
101	Nucleotide-dependent conformational states of actin. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 12723-12728.	7.1	106
102	Proton Transport Behavior through the Influenza A M2 Channel: Insights from Molecular Simulation. Biophysical Journal, 2007, 93, 3470-3479.	0.5	105
103	A Multiscale Coarse-Graining Study of the Liquid/Vacuum Interface of Room-Temperature Ionic Liquids with Alkyl Substituents of Different Lengths. Journal of Physical Chemistry C, 2008, 112, 1132-1139.	3.1	105
104	Hydrated Excess Proton at Waterâ^'Hydrophobic Interfaces. Journal of Physical Chemistry B, 2009, 113, 4017-4030.	2.6	104
105	Fascin- and Î±-Actinin-Bundled Networks Contain Intrinsic Structural Features that Drive Protein Sorting. Current Biology, 2016, 26, 2697-2706.	3.9	104
106	A Failure of Continuum Theory:â€‰ Temperature Dependence of the Solvent Reorganization Energy of Electron Transfer in Highly Polar Solvents. Journal of Physical Chemistry B, 1999, 103, 9130-9140.	2.6	103
107	Bridging Microscopic and Mesoscopic Simulations of Lipid Bilayers. Biophysical Journal, 2002, 83, 3357-3370.	0.5	103
108	On the representability problem and the physical meaning of coarse-grained models. Journal of Chemical Physics, 2016, 145, 044108.	3.0	103

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109	Factors Influencing Local Membrane Curvature Induction by N-BAR Domains as Revealed by Molecular Dynamics Simulations. Biophysical Journal, 2008, 95, 1866-1876.	0.5	102
110	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
111	Actin filament remodeling by actin depolymerization factor/cofilin. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 7299-7304.	7.1	100
112	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
113	Advances in coarse-grained modeling of macromolecular complexes. Current Opinion in Structural Biology, 2018, 52, 119-126.	5.7	100
114	Ab initio molecular-dynamics simulation of aqueous proton solvation and transport revisited. Journal of Chemical Physics, 2005, 123, 044505.	3.0	99
115	Systematic Coarse-graining of a Multicomponent Lipid Bilayer. Journal of Physical Chemistry B, 2009, 113, 1501-1510.	2.6	99
116	Ligand-Dependent Activation and Deactivation of the Human Adenosine A2A Receptor. Journal of the American Chemical Society, 2013, 135, 8749-8759.	13.7	99
117	On the amphiphilic behavior of the hydrated proton: an ab initio molecular dynamics study. International Journal of Mass Spectrometry, 2005, 241, 197-204.	1.5	97
118	Coarse-Grained Modeling of the Self-Association of Therapeutic Monoclonal Antibodies. Journal of Physical Chemistry B, 2012, 116, 8045-8057.	2.6	97
119	Simple reversible molecular dynamics algorithms for NosÃ©â€“Hoover chain dynamics. Journal of Chemical Physics, 1997, 107, 9514-9526.	3.0	95
120	Molecular Dynamics Simulation of Proton Transport Near the Surface of a Phospholipid Membrane. Biophysical Journal, 2002, 82, 1460-1468.	0.5	93
121	A centroid molecular dynamics study of liquidpara-hydrogen andortho-deuterium. Journal of Chemical Physics, 2004, 121, 6412-6422.	3.0	92
122	A Feynman path centroid dynamics approach for the computation of time correlation functions involving nonlinear operators. Journal of Chemical Physics, 2000, 113, 919-929.	3.0	91
123	Membrane Remodeling from N-BAR Domain Interactions: Insights from Multi-Scale Simulation. Biophysical Journal, 2007, 92, 3595-3602.	0.5	91
124	Molecular Dynamics Simulations of Proton Transport in 3M and Nafion Perfluorosulfonic Acid Membranes. Journal of Physical Chemistry C, 2013, 117, 8079-8091.	3.1	91
125	Modeling the free energy surfaces of electron transfer in condensed phases. Journal of Chemical Physics, 2000, 113, 5413.	3.0	90
126	Coarse-graining of multiprotein assemblies. Current Opinion in Structural Biology, 2012, 22, 144-150.	5.7	90

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127	Efficient and Minimal Method to Bias Molecular Simulations with Experimental Data. Journal of Chemical Theory and Computation, 2014, 10, 3023-3030.	5.3	90
128	Quantum-mechanical reaction rate constants from centroid molecular dynamics simulations. Journal of Chemical Physics, 2001, 115, 9209-9222.	3.0	86
129	Multiscale Coarse-Graining of Monosaccharides. Journal of Physical Chemistry B, 2007, 111, 11566-11575.	2.6	86
130	Solvent-Free Lipid Bilayer Model Using Multiscale Coarse-Graining. Journal of Physical Chemistry B, 2009, 113, 4443-4455.	2.6	86
131	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
132	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
133	A unified framework for quantum activated rate processes. I. General theory. Journal of Chemical Physics, 1996, 105, 6856-6870.	3.0	85
134	Ab initio centroid molecular dynamics: a fully quantum method for condensed-phase dynamics simulations. Chemical Physics Letters, 1999, 300, 93-98.	2.6	84
135	Elucidation of the Proton Transport Mechanism in Human Carbonic Anhydrase II. Journal of the American Chemical Society, 2009, 131, 7598-7608.	13.7	84
136	Structure and Dynamics of the Actin Filament. Journal of Molecular Biology, 2010, 396, 252-263.	4.2	84
137	Proton Transport Mechanism of Perfluorosulfonic Acid Membranes. Journal of Physical Chemistry C, 2014, 118, 17436-17445.	3.1	84
138	Peptide Folding Using Multiscale Coarse-Grained Models. Journal of Physical Chemistry B, 2008, 112, 13079-13090.	2.6	83
139	Hydrated Excess Protons Can Create Their Own Water Wires. Journal of Physical Chemistry B, 2015, 119, 9212-9218.	2.6	83
140	Classical and Quantum Simulation of Electron Transfer Through a Polypeptide. Journal of Physical Chemistry B, 1999, 103, 7367-7382.	2.6	82
141	Ab Initio Calculations of Reactive Pathways for Î±-Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (Î±-HMX). Journal of Physical Chemistry A, 2000, 104, 11384-11389.	2.5	82
142	Computer simulation of explicit proton translocation in cytochrome c oxidase: The D-pathway. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6795-6800.	7.1	82
143	Defining Coarse-Grained Representations of Large Biomolecules and Biomolecular Complexes from Elastic Network Models. Biophysical Journal, 2009, 97, 2327-2337.	0.5	82
144	Ab initiomolecular dynamics simulation of the Ag(111)-water interface. Journal of Chemical Physics, 2001, 115, 7196-7206.	3.0	81

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145	Understanding the Role of Amphipathic Helices in N-BAR Domain Driven Membrane Remodeling. Biophysical Journal, 2013, 104, 404-411.	0.5	81
146	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
147	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
148	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
149	A novel method for simulating quantum dissipative systems. Journal of Chemical Physics, 1996, 104, 4189-4197.	3.0	80
150	Mechanisms of Passive Ion Permeation through Lipid Bilayers:Â Insights from Simulations. Journal of Physical Chemistry B, 2006, 110, 21327-21337.	2.6	80
151	A path integral study of electronic polarization and nonlinear coupling effects in condensed phase proton transfer reactions. Journal of Chemical Physics, 1994, 100, 3039-3047.	3.0	79
152	Ab initio molecular dynamics simulation of the Cu(110)â€“water interface. Journal of Chemical Physics, 2001, 114, 3248-3257.	3.0	79
153	A Multi-State Empirical Valence Bond Model for Weak Acid Dissociation in Aqueous Solutionâ€. Journal of Physical Chemistry A, 2001, 105, 2814-2823.	2.5	78
154	A linear-scaling self-consistent generalization of the multistate empirical valence bond method for multiple excess protons in aqueous systems. Journal of Chemical Physics, 2005, 122, 144105.	3.0	78
155	Molecular Dynamics Simulation of the Energetic Room-Temperature Ionic Liquid, 1-Hydroxyethyl-4-amino-1,2,4-triazolium Nitrate (HEATN). Journal of Physical Chemistry B, 2008, 112, 3121-3131.	2.6	78
156	Nanostructural Organization in Acetonitrile/Ionic Liquid Mixtures: Molecular Dynamics Simulations and Optical Kerr Effect Spectroscopy. ChemPhysChem, 2012, 13, 1687-1700.	2.1	78
157	Protein-Mediated Transformation of Lipid Vesicles into Tubular Networks. Biophysical Journal, 2013, 105, 711-719.	0.5	77
158	Fitting coarse-grained distribution functions through an iterative force-matching method. Journal of Chemical Physics, 2013, 139, 121906.	3.0	77
159	Vibrational energy relaxation of Siâ€“H stretching modes on the H/Si(111)1Ã—1 surface. Journal of Chemical Physics, 1993, 99, 740-743.	3.0	76
160	The Role of Amino Acid Sequence in the Self-Association of Therapeutic Monoclonal Antibodies: Insights from Coarse-Grained Modeling. Journal of Physical Chemistry B, 2013, 117, 1269-1279.	2.6	76
161	Competition between Tropomyosin, Fimbrin, and ADF/Cofilin drives their sorting to distinct actin filament networks. ELife, 2017, 6, .	6.0	76
162	Semiclassical approximations to quantum dynamical time correlation functions. Journal of Chemical Physics, 1996, 104, 273-285.	3.0	75

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163	Transferable Coarse-Grained Models for Ionic Liquids. Journal of Chemical Theory and Computation, 2009, 5, 1091-1098.	5.3	75
164	Multiscale Computer Simulation of the Immature HIV-1 Virion. Biophysical Journal, 2010, 99, 2757-2765.	0.5	75
165	Kinetics of Proton Migration in Liquid Water. Journal of Physical Chemistry B, 2010, 114, 333-339.	2.6	75
166	New Insights into BAR Domain-Induced Membrane Remodeling. Biophysical Journal, 2009, 97, 1616-1625.	0.5	74
167	Role of Protein Interactions in Defining HIV-1 Viral Capsid Shape and Stability: A Coarse-Grained Analysis. Biophysical Journal, 2010, 98, 18-26.	0.5	74
168	Unraveling the Mystery of ATP Hydrolysis in Actin Filaments. Journal of the American Chemical Society, 2014, 136, 13053-13058.	13.7	74
169	Origins of Proton Transport Behavior from Selectivity Domain Mutations of the Aquaporin-1 Channel. Biophysical Journal, 2006, 90, L73-L75.	0.5	73
170	Infrared Spectrum of the Hydrated Proton in Water. Journal of Physical Chemistry Letters, 2011, 2, 81-86.	4.6	72
171	Pseudopotentials for centroid molecular dynamics: Application to self-diffusion in liquid para-hydrogen. Chemical Physics Letters, 1996, 249, 231-236.	2.6	71
172	Ab initio molecular dynamics: Propagating the density matrix with gaussian orbitals. IV. Formal analysis of the deviations from born-oppenheimer dynamics. Israel Journal of Chemistry, 2002, 42, 191-202.	2.3	71
173	Coupling Field Theory with Continuum Mechanics: A Simulation of Domain Formation in Giant Unilamellar Vesicles. Biophysical Journal, 2005, 88, 3855-3869.	0.5	71
174	A theory for the activated barrier crossing rate constant in systems influenced by space and time dependent friction. Journal of Chemical Physics, 1994, 101, 7811-7822.	3.0	70
175	A theory for adiabatic bond breaking electron transfer reactions at metal electrodes. Chemical Physics Letters, 1998, 282, 100-106.	2.6	70
176	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
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