

# Gregory A Voth

## List of Publications by Year in descending order

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543  
papers

42,572  
citations

2309

101  
h-index

4853

174  
g-index

596  
all docs

596  
docs citations

596  
times ranked

23834  
citing authors

#	ARTICLE	IF	CITATIONS
1	A Multiscale Coarse-Graining Method for Biomolecular Systems. <i>Journal of Physical Chemistry B</i> , 2005, 109, 2469-2473.	1.2	1,018
2	Flexible simple point-charge water model with improved liquid-state properties. <i>Journal of Chemical Physics</i> , 2006, 124, 024503.	1.2	955
3	Unique Spatial Heterogeneity in Ionic Liquids. <i>Journal of the American Chemical Society</i> , 2005, 127, 12192-12193.	6.6	919
4	The multiscale coarse-graining method. I. A rigorous bridge between atomistic and coarse-grained models. <i>Journal of Chemical Physics</i> , 2008, 128, 244114.	1.2	651
5	On the Structure and Dynamics of Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2004, 108, 1744-1752.	1.2	649
6	The computer simulation of proton transport in water. <i>Journal of Chemical Physics</i> , 1999, 111, 9361-9381.	1.2	557
7	Multiscale coarse graining of liquid-state systems. <i>Journal of Chemical Physics</i> , 2005, 123, 134105.	1.2	531
8	Rigorous formulation of quantum transition state theory and its dynamical corrections. <i>Journal of Chemical Physics</i> , 1989, 91, 7749-7760.	1.2	498
9	Coarse-Graining Methods for Computational Biology. <i>Annual Review of Biophysics</i> , 2013, 42, 73-93.	4.5	475
10	The formulation of quantum statistical mechanics based on the Feynman path centroid density. II. Dynamical properties. <i>Journal of Chemical Physics</i> , 1994, 100, 5106-5117.	1.2	454
11	Molecular Dynamics Simulation of Nanostructural Organization in Ionic Liquid/Water Mixtures. <i>Journal of Physical Chemistry B</i> , 2007, 111, 4812-4818.	1.2	431
12	Ab initio molecular dynamics: Propagating the density matrix with Gaussian orbitals. III. Comparison with Born-Oppenheimer dynamics. <i>Journal of Chemical Physics</i> , 2002, 117, 8694-8704.	1.2	430
13	Multistate Empirical Valence Bond Model for Proton Transport in Water. <i>Journal of Physical Chemistry B</i> , 1998, 102, 5547-5551.	1.2	397
14	Computer Simulation of Proton Solvation and Transport in Aqueous and Biomolecular Systems. <i>Accounts of Chemical Research</i> , 2006, 39, 143-150.	7.6	395
15	Multiscale modeling of biomolecular systems: in serial and in parallel. <i>Current Opinion in Structural Biology</i> , 2007, 17, 192-198.	2.6	395
16	Molecular Dynamics Simulation of Ionic Liquids: The Effect of Electronic Polarizability. <i>Journal of Physical Chemistry B</i> , 2004, 108, 11877-11881.	1.2	393
17	Tail Aggregation and Domain Diffusion in Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2006, 110, 18601-18608.	1.2	387
18	Effective force fields for condensed phase systems from ab initio molecular dynamics simulation: A new method for force-matching. <i>Journal of Chemical Physics</i> , 2004, 120, 10896-10913.	1.2	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. <i>Journal of Chemical Physics</i> , 2001, 115, 10291.	1.2	375
20	The quantum dynamics of an excess proton in water. <i>Journal of Chemical Physics</i> , 1996, 104, 2056-2069.	1.2	328
21	The multiscale coarse-graining method. II. Numerical implementation for coarse-grained molecular models. <i>Journal of Chemical Physics</i> , 2008, 128, 244115.	1.2	326
22	Understanding Ionic Liquids through Atomistic and Coarse-Grained Molecular Dynamics Simulations. <i>Accounts of Chemical Research</i> , 2007, 40, 1193-1199.	7.6	304
23	The formulation of quantum statistical mechanics based on the Feynman path centroid density. IV. Algorithms for centroid molecular dynamics. <i>Journal of Chemical Physics</i> , 1994, 101, 6168-6183.	1.2	299
24	The formulation of quantum statistical mechanics based on the Feynman path centroid density. I. Equilibrium properties. <i>Journal of Chemical Physics</i> , 1994, 100, 5093-5105.	1.2	298
25	Special Pair Dance and Partner Selection: Elementary Steps in Proton Transport in Liquid Water. <i>Journal of Physical Chemistry B</i> , 2008, 112, 9456-9466.	1.2	291
26	A second generation multistate empirical valence bond model for proton transport in aqueous systems. <i>Journal of Chemical Physics</i> , 2002, 117, 5839-5849.	1.2	285
27	Proton Solvation and Transport in Aqueous and Biomolecular Systems: Insights from Computer Simulations. <i>Journal of Physical Chemistry B</i> , 2007, 111, 4300-4314.	1.2	279
28	The Curious Case of the Hydrated Proton. <i>Accounts of Chemical Research</i> , 2012, 45, 101-109.	7.6	266
29	A derivation of centroid molecular dynamics and other approximate time evolution methods for path integral centroid variables. <i>Journal of Chemical Physics</i> , 1999, 111, 2371-2384.	1.2	261
30	Ionic Liquids. <i>Accounts of Chemical Research</i> , 2007, 40, 1077-1078.	7.6	259
31	The Hydrated Proton at the Water Liquid/Vapor Interface. <i>Journal of Physical Chemistry B</i> , 2004, 108, 14804-14806.	1.2	255
32	Well-Tempered Metadynamics Converges Asymptotically. <i>Physical Review Letters</i> , 2014, 112, 240602.	2.9	248
33	When Physics Takes Over: BAR Proteins and Membrane Curvature. <i>Trends in Cell Biology</i> , 2015, 25, 780-792.	3.6	247
34	Further developments in the local-orbital density-functional-theory tight-binding method. <i>Physical Review B</i> , 2001, 64, .	1.1	232
35	Mixed Atomistic and Coarse-Grained Molecular Dynamics: A Simulation of a Membrane-Bound Ion Channel. <i>Journal of Physical Chemistry B</i> , 2006, 110, 15045-15048.	1.2	230
36	A bond-order analysis of the mechanism for hydrated proton mobility in liquid water. <i>Journal of Chemical Physics</i> , 2005, 122, 014506.	1.2	229

#	ARTICLE	IF	CITATIONS
37	An Improved Multistate Empirical Valence Bond Model for Aqueous Proton Solvation and Transport. <i>Journal of Physical Chemistry B</i> , 2008, 112, 467-482.	1.2	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. <i>Journal of Chemical Physics</i> , 1994, 101, 6157-6167.	1.2	225
39	A new perspective on quantum time correlation functions. <i>Journal of Chemical Physics</i> , 1993, 99, 10070-10073.	1.2	224
40	Structural Basis of Membrane Bending by the N-BAR Protein Endophilin. <i>Cell</i> , 2012, 149, 137-145.	13.5	220
41	Direct observation of Bin/amphiphysin/Rvs (BAR) domain-induced membrane curvature by means of molecular dynamics simulations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 15068-15072.	3.3	218
42	The 2018 biomembrane curvature and remodeling roadmap. <i>Journal Physics D: Applied Physics</i> , 2018, 51, 343001.	1.3	212
43	Hydroxide Solvation and Transport in Anion Exchange Membranes. <i>Journal of the American Chemical Society</i> , 2016, 138, 991-1000.	6.6	208
44	The vibrational spectrum of the hydrated proton: Comparison of experiment, simulation, and normal mode analysis. <i>Journal of Chemical Physics</i> , 2002, 116, 737-746.	1.2	200
45	The Properties of Water: Insights from Quantum Simulations. <i>Journal of Physical Chemistry B</i> , 2009, 113, 5702-5719.	1.2	199
46	Structure of the Liquid-Vacuum Interface of Room-Temperature Ionic Liquids: A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 1800-1806.	1.2	195
47	Multiscale Coarse-Graining and Structural Correlations: Connections to Liquid-State Theory. <i>Journal of Physical Chemistry B</i> , 2007, 111, 4116-4127.	1.2	191
48	Path integral centroid variables and the formulation of their exact real time dynamics. <i>Journal of Chemical Physics</i> , 1999, 111, 2357-2370.	1.2	190
49	A quantum model for water: Equilibrium and dynamical properties. <i>Journal of Chemical Physics</i> , 1997, 106, 2400-2410.	1.2	187
50	An accurate and simple quantum model for liquid water. <i>Journal of Chemical Physics</i> , 2006, 125, 184507.	1.2	187
51	Modeling real dynamics in the coarse-grained representation of condensed phase systems. <i>Journal of Chemical Physics</i> , 2006, 125, 151101.	1.2	184
52	Mechanism of Membrane Curvature Sensing by Amphipathic Helix Containing Proteins. <i>Biophysical Journal</i> , 2011, 100, 1271-1279.	0.2	184
53	Molecular dynamics simulations of imidazolium-based ionic liquid/water mixtures: Alkyl side chain length and anion effects. <i>Fluid Phase Equilibria</i> , 2010, 294, 148-156.	1.4	182
54	The Mechanism of Hydrated Proton Transport in Water. <i>Journal of the American Chemical Society</i> , 2000, 122, 12027-12028.	6.6	180

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55	The Formation and Dynamics of Proton Wires in Channel Environments. <i>Biophysical Journal</i> , 2001, 80, 1691-1702.	0.2	178
56	Allostery of actin filaments: Molecular dynamics simulations and coarse-grained analysis. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 13111-13116.	3.3	178
57	Coarse-Grained Modeling of the Actin Filament Derived from Atomistic-Scale Simulations. <i>Biophysical Journal</i> , 2006, 90, 1572-1582.	0.2	178
58	Coarse-Grained Peptide Modeling Using a Systematic Multiscale Approach. <i>Biophysical Journal</i> , 2007, 92, 4289-4303.	0.2	176
59	Mechanism and Determinants of Amphipathic Helix-Containing Protein Targeting to Lipid Droplets. <i>Developmental Cell</i> , 2018, 44, 73-86.e4.	3.1	175
60	Transition State Dynamics and Relaxation Processes in Solutions: A Frontier of Physical Chemistry. <i>The Journal of Physical Chemistry</i> , 1996, 100, 13034-13049.	2.9	174
61	Multiscale Coarse-Graining of Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2006, 110, 3564-3575.	1.2	174
62	Characterization of the Solvation and Transport of the Hydrated Proton in the Perfluorosulfonic Acid Membrane Nafion. <i>Journal of Physical Chemistry B</i> , 2006, 110, 18594-18600.	1.2	171
63	Friction Mediates Scission of Tubular Membranes Scaffolded by BAR Proteins. <i>Cell</i> , 2017, 170, 172-184.e11.	13.5	171
64	A Systematic Methodology for Defining Coarse-Grained Sites in Large Biomolecules. <i>Biophysical Journal</i> , 2008, 95, 5073-5083.	0.2	153
65	The Theory of Electron Transfer Reactions: What May Be Missing?. <i>Journal of the American Chemical Society</i> , 2003, 125, 7470-7478.	6.6	152
66	Quantum effects in liquid water from an <i>ab initio</i> -based polarizable force field. <i>Journal of Chemical Physics</i> , 2007, 127, 074506.	1.2	151
67	The Theory of Ultra-Coarse-Graining. 1. General Principles. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2466-2480.	2.3	149
68	The mechanism of proton exclusion in aquaporin channels. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 55, 223-228.	1.5	148
69	Systematic Multiscale Parameterization of Heterogeneous Elastic Network Models of Proteins. <i>Biophysical Journal</i> , 2008, 95, 4183-4192.	0.2	148
70	Path-Integral Centroid Methods in Quantum Statistical Mechanics and Dynamics. <i>Advances in Chemical Physics</i> , 2007, , 135-218.	0.3	145
71	Mechanism of Fast Proton Transport along One-Dimensional Water Chains Confined in Carbon Nanotubes. <i>Journal of the American Chemical Society</i> , 2010, 132, 11395-11397.	6.6	144
72	Linear aggregation of proteins on the membrane as a prelude to membrane remodeling. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 20396-20401.	3.3	144

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73	Proton Transfer in the Enzyme Carbonic Anhydrase: An Ab Initio Study. <i>Journal of the American Chemical Society</i> , 1998, 120, 4006-4014.	6.6	143
74	Membrane tension controls the assembly of curvature-generating proteins. <i>Nature Communications</i> , 2015, 6, 7219.	5.8	141
75	A multiscale coarse-grained model of the SARS-CoV-2 virion. <i>Biophysical Journal</i> , 2021, 120, 1097-1104.	0.2	139
76	Multiscale Coarse-Graining of Mixed Phospholipid/Cholesterol Bilayers. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 637-648.	2.3	138
77	Atomistic Modeling of the Electrode-Electrolyte Interface in Li-Ion Energy Storage Systems: Electrolyte Structuring. <i>Journal of Physical Chemistry C</i> , 2013, 117, 3747-3761.	1.5	137
78	Coarse-grained simulation reveals key features of HIV-1 capsid self-assembly. <i>Nature Communications</i> , 2016, 7, 11568.	5.8	134
79	Hybrid Ab-Initio/Empirical Molecular Dynamics: Combining the ONIOM Scheme with the Atom-Centered Density Matrix Propagation (ADMP) Approach. <i>Journal of Physical Chemistry B</i> , 2004, 108, 4210-4220.	1.2	131
80	A comparative study of imaginary time path integral based methods for quantum dynamics. <i>Journal of Chemical Physics</i> , 2006, 124, 154103.	1.2	131
81	Exact exchange in ab initio molecular dynamics: An efficient plane-wave based algorithm. <i>Journal of Chemical Physics</i> , 1998, 108, 4697-4700.	1.2	130
82	Probing Selected Morphological Models of Hydrated Nafion Using Large-Scale Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2010, 114, 3205-3218.	1.2	129
83	Proton Solvation and Transport in Hydrated Nafion. <i>Journal of Physical Chemistry B</i> , 2011, 115, 5903-5912.	1.2	125
84	Coarse-Grained Free Energy Functions for Studying Protein Conformational Changes: A Double-Well Network Model. <i>Biophysical Journal</i> , 2007, 93, 3860-3871.	0.2	124
85	Effective force coarse-graining. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 2002.	1.3	124
86	Infrared Spectroscopy and Hydrogen-Bond Dynamics of Liquid Water from Centroid Molecular Dynamics with an Ab Initio-Based Force Field. <i>Journal of Physical Chemistry B</i> , 2009, 113, 13118-13130.	1.2	123
87	Excess Proton Solvation and Delocalization in a Hydrophilic Pocket of the Proton Conducting Polymer Membrane Nafion. <i>Journal of Physical Chemistry B</i> , 2005, 109, 3727-3730.	1.2	122
88	Applications of higher order composite factorization schemes in imaginary time path integral simulations. <i>Journal of Chemical Physics</i> , 2001, 115, 7832-7842.	1.2	120
89	How curvature-generating proteins build scaffolds on membrane nanotubes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 11226-11231.	3.3	120
90	The formulation of quantum statistical mechanics based on the Feynman path centroid density. V. Quantum instantaneous normal mode theory of liquids. <i>Journal of Chemical Physics</i> , 1994, 101, 6184-6192.	1.2	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. <i>Structure</i> , 2009, 17, 1660-1668.	1.6	118
92	Multiscale Coarse-Graining of the Protein Energy Landscape. <i>PLoS Computational Biology</i> , 2010, 6, e1000827.	1.5	116
93	Charge Delocalization in Proton Channels, I: The Aquaporin Channels and Proton Blockage. <i>Biophysical Journal</i> , 2007, 92, 46-60.	0.2	114
94	The multiscale coarse-graining method. VI. Implementation of three-body coarse-grained potentials. <i>Journal of Chemical Physics</i> , 2010, 132, 164107.	1.2	113
95	Calculation of solvent free energies for heterogeneous electron transfer at the water-metal interface: Classical versus quantum behavior. <i>Journal of Chemical Physics</i> , 1995, 102, 529-539.	1.2	112
96	Molecular Dynamics Simulation of Proton Transport through the Influenza A Virus M2 Channel. <i>Biophysical Journal</i> , 2002, 83, 1987-1996.	0.2	111
97	Efficient, Regularized, and Scalable Algorithms for Multiscale Coarse-Graining. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 954-965.	2.3	110
98	Systematic Coarse-Graining of Nanoparticle Interactions in Molecular Dynamics Simulation. <i>Journal of Physical Chemistry B</i> , 2005, 109, 17019-17024.	1.2	109
99	The multiscale coarse-graining method. IV. Transferring coarse-grained potentials between temperatures. <i>Journal of Chemical Physics</i> , 2009, 131, 024103.	1.2	108
100	Car Parrinello molecular dynamics simulation of liquid water: New results. <i>Journal of Chemical Physics</i> , 2002, 116, 10372-10376.	1.2	106
101	Nucleotide-dependent conformational states of actin. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 12723-12728.	3.3	106
102	Proton Transport Behavior through the Influenza A M2 Channel: Insights from Molecular Simulation. <i>Biophysical Journal</i> , 2007, 93, 3470-3479.	0.2	105
103	A Multiscale Coarse-Graining Study of the Liquid/Vacuum Interface of Room-Temperature Ionic Liquids with Alkyl Substituents of Different Lengths. <i>Journal of Physical Chemistry C</i> , 2008, 112, 1132-1139.	1.5	105
104	Hydrated Excess Proton at Water-Hydrophobic Interfaces. <i>Journal of Physical Chemistry B</i> , 2009, 113, 4017-4030.	1.2	104
105	Fascin- and $\hat{\pm}$ -Actinin-Bundled Networks Contain Intrinsic Structural Features that Drive Protein Sorting. <i>Current Biology</i> , 2016, 26, 2697-2706.	1.8	104
106	A Failure of Continuum Theory: Temperature Dependence of the Solvent Reorganization Energy of Electron Transfer in Highly Polar Solvents. <i>Journal of Physical Chemistry B</i> , 1999, 103, 9130-9140.	1.2	103
107	Bridging Microscopic and Mesoscopic Simulations of Lipid Bilayers. <i>Biophysical Journal</i> , 2002, 83, 3357-3370.	0.2	103
108	On the representability problem and the physical meaning of coarse-grained models. <i>Journal of Chemical Physics</i> , 2016, 145, 044108.	1.2	103

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109	Factors Influencing Local Membrane Curvature Induction by N-BAR Domains as Revealed by Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2008, 95, 1866-1876.	0.2	102
110	Lamellipodium is a myosin-independent mechanosensor. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 2646-2651.	3.3	101
111	Actin filament remodeling by actin depolymerization factor/cofilin. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 7299-7304.	3.3	100
112	Propensity of Hydrated Excess Protons and Hydroxide Anions for the Air-Water Interface. <i>Journal of the American Chemical Society</i> , 2015, 137, 12610-12616.	6.6	100
113	Advances in coarse-grained modeling of macromolecular complexes. <i>Current Opinion in Structural Biology</i> , 2018, 52, 119-126.	2.6	100
114	Ab initio molecular-dynamics simulation of aqueous proton solvation and transport revisited. <i>Journal of Chemical Physics</i> , 2005, 123, 044505.	1.2	99
115	Systematic Coarse-graining of a Multicomponent Lipid Bilayer. <i>Journal of Physical Chemistry B</i> , 2009, 113, 1501-1510.	1.2	99
116	Ligand-Dependent Activation and Deactivation of the Human Adenosine A2A Receptor. <i>Journal of the American Chemical Society</i> , 2013, 135, 8749-8759.	6.6	99
117	On the amphiphilic behavior of the hydrated proton: an ab initio molecular dynamics study. <i>International Journal of Mass Spectrometry</i> , 2005, 241, 197-204.	0.7	97
118	Coarse-Grained Modeling of the Self-Association of Therapeutic Monoclonal Antibodies. <i>Journal of Physical Chemistry B</i> , 2012, 116, 8045-8057.	1.2	97
119	Simple reversible molecular dynamics algorithms for Nosé-Hoover chain dynamics. <i>Journal of Chemical Physics</i> , 1997, 107, 9514-9526.	1.2	95
120	Molecular Dynamics Simulation of Proton Transport Near the Surface of a Phospholipid Membrane. <i>Biophysical Journal</i> , 2002, 82, 1460-1468.	0.2	93
121	A centroid molecular dynamics study of liquid para-hydrogen and ortho-deuterium. <i>Journal of Chemical Physics</i> , 2004, 121, 6412-6422.	1.2	92
122	A Feynman path centroid dynamics approach for the computation of time correlation functions involving nonlinear operators. <i>Journal of Chemical Physics</i> , 2000, 113, 919-929.	1.2	91
123	Membrane Remodeling from N-BAR Domain Interactions: Insights from Multi-Scale Simulation. <i>Biophysical Journal</i> , 2007, 92, 3595-3602.	0.2	91
124	Molecular Dynamics Simulations of Proton Transport in 3M and Nafion Perfluorosulfonic Acid Membranes. <i>Journal of Physical Chemistry C</i> , 2013, 117, 8079-8091.	1.5	91
125	Modeling the free energy surfaces of electron transfer in condensed phases. <i>Journal of Chemical Physics</i> , 2000, 113, 5413.	1.2	90
126	Coarse-graining of multiprotein assemblies. <i>Current Opinion in Structural Biology</i> , 2012, 22, 144-150.	2.6	90



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127	Efficient and Minimal Method to Bias Molecular Simulations with Experimental Data. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3023-3030.	2.3	90
128	Quantum-mechanical reaction rate constants from centroid molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2001, 115, 9209-9222.	1.2	86
129	Multiscale Coarse-Graining of Monosaccharides. <i>Journal of Physical Chemistry B</i> , 2007, 111, 11566-11575.	1.2	86
130	Solvent-Free Lipid Bilayer Model Using Multiscale Coarse-Graining. <i>Journal of Physical Chemistry B</i> , 2009, 113, 4443-4455.	1.2	86
131	Dynamic force matching: A method for constructing dynamical coarse-grained models with realistic time dependence. <i>Journal of Chemical Physics</i> , 2015, 142, 154104.	1.2	86
132	Immature HIV-1 lattice assembly dynamics are regulated by scaffolding from nucleic acid and the plasma membrane. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E10056-E10065.	3.3	86
133	A unified framework for quantum activated rate processes. I. General theory. <i>Journal of Chemical Physics</i> , 1996, 105, 6856-6870.	1.2	85
134	Ab initio centroid molecular dynamics: a fully quantum method for condensed-phase dynamics simulations. <i>Chemical Physics Letters</i> , 1999, 300, 93-98.	1.2	84
135	Elucidation of the Proton Transport Mechanism in Human Carbonic Anhydrase II. <i>Journal of the American Chemical Society</i> , 2009, 131, 7598-7608.	6.6	84
136	Structure and Dynamics of the Actin Filament. <i>Journal of Molecular Biology</i> , 2010, 396, 252-263.	2.0	84
137	Proton Transport Mechanism of Perfluorosulfonic Acid Membranes. <i>Journal of Physical Chemistry C</i> , 2014, 118, 17436-17445.	1.5	84
138	Peptide Folding Using Multiscale Coarse-Grained Models. <i>Journal of Physical Chemistry B</i> , 2008, 112, 13079-13090.	1.2	83
139	Hydrated Excess Protons Can Create Their Own Water Wires. <i>Journal of Physical Chemistry B</i> , 2015, 119, 9212-9218.	1.2	83
140	Classical and Quantum Simulation of Electron Transfer Through a Polypeptide. <i>Journal of Physical Chemistry B</i> , 1999, 103, 7367-7382.	1.2	82
141	Ab Initio Calculations of Reactive Pathways for $\hat{I}^{\pm}$ -Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine ( $\hat{I}^{\pm}$ -HMX). <i>Journal of Physical Chemistry A</i> , 2000, 104, 11384-11389.	1.1	82
142	Computer simulation of explicit proton translocation in cytochrome c oxidase: The D-pathway. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 6795-6800.	3.3	82
143	Defining Coarse-Grained Representations of Large Biomolecules and Biomolecular Complexes from Elastic Network Models. <i>Biophysical Journal</i> , 2009, 97, 2327-2337.	0.2	82
144	Ab initiomolecular dynamics simulation of the Ag(111)-water interface. <i>Journal of Chemical Physics</i> , 2001, 115, 7196-7206.	1.2	81

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145	Understanding the Role of Amphipathic Helices in N-BAR Domain Driven Membrane Remodeling. <i>Biophysical Journal</i> , 2013, 104, 404-411.	0.2	81
146	Multiscale simulation reveals a multifaceted mechanism of proton permeation through the influenza A M2 proton channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 9396-9401.	3.3	81
147	Acid activation mechanism of the influenza A M2 proton channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, E6955-E6964.	3.3	81
148	Proton movement and coupling in the POT family of peptide transporters. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 13182-13187.	3.3	81
149	A novel method for simulating quantum dissipative systems. <i>Journal of Chemical Physics</i> , 1996, 104, 4189-4197.	1.2	80
150	Mechanisms of Passive Ion Permeation through Lipid Bilayers: Insights from Simulations. <i>Journal of Physical Chemistry B</i> , 2006, 110, 21327-21337.	1.2	80
151	A path integral study of electronic polarization and nonlinear coupling effects in condensed phase proton transfer reactions. <i>Journal of Chemical Physics</i> , 1994, 100, 3039-3047.	1.2	79
152	Ab initio molecular dynamics simulation of the Cu(110)–water interface. <i>Journal of Chemical Physics</i> , 2001, 114, 3248-3257.	1.2	79
153	A Multi-State Empirical Valence Bond Model for Weak Acid Dissociation in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 2001, 105, 2814-2823.	1.1	78
154	A linear-scaling self-consistent generalization of the multistate empirical valence bond method for multiple excess protons in aqueous systems. <i>Journal of Chemical Physics</i> , 2005, 122, 144105.	1.2	78
155	Molecular Dynamics Simulation of the Energetic Room-Temperature Ionic Liquid, 1-Hydroxyethyl-4-amino-1,2,4-triazolium Nitrate (HEATN). <i>Journal of Physical Chemistry B</i> , 2008, 112, 3121-3131.	1.2	78
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157	Protein-Mediated Transformation of Lipid Vesicles into Tubular Networks. <i>Biophysical Journal</i> , 2013, 105, 711-719.	0.2	77
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