Gregory A Voth

List of Publications by Citations

536 papers	36,352 citations	96 h-index	164 g-index
596 ext. papers	39,725 ext. citations	5.3 avg, IF	7.85 L-index

#	Paper	IF	Citations
536	A multiscale coarse-graining method for biomolecular systems. *Journal of Physical Chemistry B*, **2005**, 109, 2469-73	3.4	879
535	Unique spatial heterogeneity in ionic liquids. *Journal of the American Chemical Society*, **2005**, 127, 12192-3	12.4	853
534	Flexible simple point-charge water model with improved liquid-state properties. *Journal of Chemical Physics*, **2006**, 124, 024503	3.9	742
533	On the Structure and Dynamics of Ionic Liquids. *Journal of Physical Chemistry B*, **2004**, 108, 1744-1752	3.4	599
532	The multiscale coarse-graining method. I. A rigorous bridge between atomistic and coarse-grained models. *Journal of Chemical Physics*, **2008**, 128, 244114	3.9	550
531	The computer simulation of proton transport in water. *Journal of Chemical Physics*, **1999**, 111, 9361-9381	3.9	515
530	Multiscale coarse graining of liquid-state systems. *Journal of Chemical Physics*, **2005**, 123, 134105	3.9	467
529	Rigorous formulation of quantum transition state theory and its dynamical corrections. *Journal of Chemical Physics*, **1989**, 91, 7749-7760	3.9	448
528	The formulation of quantum statistical mechanics based on the Feynman path centroid density. II. Dynamical properties. *Journal of Chemical Physics*, **1994**, 100, 5106-5117	3.9	399
527	Molecular dynamics simulation of nanostructural organization in ionic liquid/water mixtures. *Journal of Physical Chemistry B*, **2007**, 111, 4812-8	3.4	395
526	Multistate Empirical Valence Bond Model for Proton Transport in Water. *Journal of Physical Chemistry B*, **1998**, 102, 5547-5551	3.4	376
525	Coarse-graining methods for computational biology. *Annual Review of Biophysics*, **2013**, 42, 73-93	21.1	373
524	Molecular Dynamics Simulation of Ionic Liquids: The Effect of Electronic Polarizability. *Journal of Physical Chemistry B*, **2004**, 108, 11877-11881	3.4	367
523	Computer simulation of proton solvation and transport in aqueous and biomolecular systems. *Accounts of Chemical Research*, **2006**, 39, 143-50	24.3	365
522	Tail aggregation and domain diffusion in ionic liquids. *Journal of Physical Chemistry B*, **2006**, 110, 18601-8	3.4	365
521	Ab initio molecular dynamics: Propagating the density matrix with Gaussian orbitals. III. Comparison with Born□Oppenheimer dynamics. *Journal of Chemical Physics*, **2002**, 117, 8694-8704	3.9	361
520	Multiscale modeling of biomolecular systems: in serial and in parallel. *Current Opinion in Structural Biology*, **2007**, 17, 192-8	8.1	359

519	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, 10896-913	3.9	349
518	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	3.9	320
517	The quantum dynamics of an excess proton in water. *Journal of Chemical Physics*, **1996**, 104, 2056-2069	3.9	314
516	Understanding ionic liquids through atomistic and coarse-grained molecular dynamics simulations. *Accounts of Chemical Research*, **2007**, 40, 1193-9	24.3	285
515	The multiscale coarse-graining method. II. Numerical implementation for coarse-grained molecular models. *Journal of Chemical Physics*, **2008**, 128, 244115	3.9	284
514	The formulation of quantum statistical mechanics based on the Feynman path centroid density. I. Equilibrium properties. *Journal of Chemical Physics*, **1994**, 100, 5093-5105	3.9	273
513	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	3.9	268
512	A second generation multistate empirical valence bond model for proton transport in aqueous systems. *Journal of Chemical Physics*, **2002**, 117, 5839-5849	3.9	266
511	Special pair dance and partner selection: elementary steps in proton transport in liquid water. *Journal of Physical Chemistry B*, **2008**, 112, 9456-66	3.4	263
510	Proton solvation and transport in aqueous and biomolecular systems: insights from computer simulations. *Journal of Physical Chemistry B*, **2007**, 111, 4300-14	3.4	260
509	Ionic liquids. *Accounts of Chemical Research*, **2007**, 40, 1077-8	24.3	243
508	The Hydrated Proton at the Water Liquid/Vapor Interface. *Journal of Physical Chemistry B*, **2004**, 108, 14804-14806	3.4	237
507	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	3.9	230
506	Further developments in the local-orbital density-functional-theory tight-binding method. *Physical Review B*, **2001**, 64,	3.3	222
505	The curious case of the hydrated proton. *Accounts of Chemical Research*, **2012**, 45, 101-9	24.3	215
504	Mixed atomistic and coarse-grained molecular dynamics: simulation of a membrane-bound ion channel. *Journal of Physical Chemistry B*, **2006**, 110, 15045-8	3.4	213
503	A bond-order analysis of the mechanism for hydrated proton mobility in liquid water. *Journal of Chemical Physics*, **2005**, 122, 14506	3.9	212
502	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	3.9	209

501	A new perspective on quantum time correlation functions. *Journal of Chemical Physics*, **1993**, 99, 10070-10073	3.9	204
500	An improved multistate empirical valence bond model for aqueous proton solvation and transport. *Journal of Physical Chemistry B*, **2008**, 112, 467-82	3.4	203
499	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, 15068-72	11.5	196
498	The vibrational spectrum of the hydrated proton: Comparison of experiment, simulation, and normal mode analysis. *Journal of Chemical Physics*, **2002**, 116, 737-746	3.9	189
497	Structural basis of membrane bending by the N-BAR protein endophilin. *Cell*, **2012**, 149, 137-45	56.2	188
496	The properties of water: insights from quantum simulations. *Journal of Physical Chemistry B*, **2009**, 113, 5702-19	3.4	187
495	Structure of the liquid-vacuum interface of room-temperature ionic liquids: a molecular dynamics study. *Journal of Physical Chemistry B*, **2006**, 110, 1800-6	3.4	185
494	When Physics Takes Over: BAR Proteins and Membrane Curvature. *Trends in Cell Biology*, **2015**, 25, 780-792	12.3	183
493	Well-tempered metadynamics converges asymptotically. *Physical Review Letters*, **2014**, 112, 240602	7.4	182
492	Path integral centroid variables and the formulation of their exact real time dynamics. *Journal of Chemical Physics*, **1999**, 111, 2357-2370	3.9	178
491	A quantum model for water: Equilibrium and dynamical properties. *Journal of Chemical Physics*, **1997**, 106, 2400-2410	3.9	176
490	The formation and dynamics of proton wires in channel environments. *Biophysical Journal*, **2001**, 80, 1691-702	3.9	169
489	An accurate and simple quantum model for liquid water. *Journal of Chemical Physics*, **2006**, 125, 184507	3.9	165
488	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	164
487	Coarse-grained modeling of the actin filament derived from atomistic-scale simulations. *Biophysical Journal*, **2006**, 90, 1572-82	2.9	161
486	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, 13111-6	11.5	161
485	The Mechanism of Hydrated Proton Transport in Water. *Journal of the American Chemical Society*, **2000**, 122, 12027-12028	16.4	161
484	Coarse-grained peptide modeling using a systematic multiscale approach. *Biophysical Journal*, **2007**, 92, 4289-303	2.9	160

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481	Transition State Dynamics and Relaxation Processes in Solutions: A Frontier of Physical Chemistry. *The Journal of Physical Chemistry*, **1996**, 100, 13034-13049		159
480	Multiscale coarse-graining of ionic liquids. *Journal of Physical Chemistry B*, **2006**, 110, 3564-75	3.4	158
479	Characterization of the solvation and transport of the hydrated proton in the perfluorosulfonic acid membrane nafion. *Journal of Physical Chemistry B*, **2006**, 110, 18594-600	3.4	156
478	Hydroxide Solvation and Transport in Anion Exchange Membranes. *Journal of the American Chemical Society*, **2016**, 138, 991-1000	16.4	155
477	Mechanism of membrane curvature sensing by amphipathic helix containing proteins. *Biophysical Journal*, **2011**, 100, 1271-9	2.9	147
476	Quantum effects in liquid water from an ab initio-based polarizable force field. *Journal of Chemical Physics*, **2007**, 127, 074506	3.9	142
475	The theory of electron transfer reactions: what may be missing?. *Journal of the American Chemical Society*, **2003**, 125, 7470-8	16.4	138
474	Proton Transfer in the Enzyme Carbonic Anhydrase: An ab Initio Study. *Journal of the American Chemical Society*, **1998**, 120, 4006-4014	16.4	138
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472	The 2018 biomembrane curvature and remodeling roadmap. *Journal Physics D: Applied Physics*, **2018**, 51,	3	133
471	Path-Integral Centroid Methods in Quantum Statistical Mechanics and Dynamics. *Advances in Chemical Physics*, **2007**, 135-218		133
470	Multiscale Coarse-Graining of Mixed Phospholipid/Cholesterol Bilayers. *Journal of Chemical Theory and Computation*, **2006**, 2, 637-48	6.4	133
469	Mechanism of fast proton transport along one-dimensional water chains confined in carbon nanotubes. *Journal of the American Chemical Society*, **2010**, 132, 11395-7	16.4	130
468	Friction Mediates Scission of Tubular Membranes Scaffolded by BAR Proteins. *Cell*, **2017**, 170, 172-184.e11	36.2	128
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458	The Theory of Ultra-Coarse-Graining. 1. General Principles. *Journal of Chemical Theory and Computation*, **2013**, 9, 2466-80	6.4	114
457	Applications of higher order composite factorization schemes in imaginary time path integral simulations. *Journal of Chemical Physics*, **2001**, 115, 7832-7842	3.9	113
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