

Daniel M Zuckerman

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

101
papers

3,492
citations

35
h-index

57
g-index

133
ext. papers

4,110
ext. citations

5.1
avg, IF

5.83
L-index

#	Paper	IF	Citations
101	Quantifying uncertainty and sampling quality in biomolecular simulations. <i>Annual Reports in Computational Chemistry</i> , 2009 , 5, 23-48	1.8	216
100	Equilibrium sampling in biomolecular simulations. <i>Annual Review of Biophysics</i> , 2011 , 40, 41-62	21.1	171
99	Resolution exchange simulation. <i>Physical Review Letters</i> , 2006 , 96, 028105	7.4	167
98	Theory of a systematic computational error in free energy differences. <i>Physical Review Letters</i> , 2002 , 89, 180602	7.4	130
97	The "weighted ensemble" path sampling method is statistically exact for a broad class of stochastic processes and binning procedures. <i>Journal of Chemical Physics</i> , 2010 , 132, 054107	3.9	122
96	Comparison of free energy methods for molecular systems. <i>Journal of Chemical Physics</i> , 2006 , 125, 184134	3.9	115
95	Weighted Ensemble Simulation: Review of Methodology, Applications, and Software. <i>Annual Review of Biophysics</i> , 2017 , 46, 43-57	21.1	101
94	Efficient and verified simulation of a path ensemble for conformational change in a united-residue model of calmodulin. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007 , 104, 18043-8	11.5	101
93	Ensemble-based convergence analysis of biomolecular trajectories. <i>Biophysical Journal</i> , 2006 , 91, 164-72	2.9	95
92	Single-ensemble nonequilibrium path-sampling estimates of free energy differences. <i>Journal of Chemical Physics</i> , 2004 , 120, 10876-9	3.9	94
91	A Second Look at Canonical Sampling of Biomolecules using Replica Exchange Simulation. <i>Journal of Chemical Theory and Computation</i> , 2006 , 2, 12001202	6.4	84
90	Transition-event durations in one-dimensional activated processes. <i>Journal of Chemical Physics</i> , 2007 , 126, 074504	3.9	79
89	Hydrophobic Matching Mechanism Investigated by Molecular Dynamics Simulations. <i>Langmuir</i> , 2002 , 18, 1340-1351	4	79
88	Dynamic reaction paths and rates through importance-sampled stochastic dynamics. <i>Journal of Chemical Physics</i> , 1999 , 111, 9475-9484	3.9	78
87	Simulation of an Ensemble of Conformational Transitions in a United-Residue Model of Calmodulin. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 5127-5137	3.4	77
86	WESTPA: an interoperable, highly scalable software package for weighted ensemble simulation and analysis. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 800-9	6.4	75
85	Efficient use of nonequilibrium measurement to estimate free energy differences for molecular systems. <i>Journal of Computational Chemistry</i> , 2004 , 25, 1749-59	3.5	67

84	Resolution Exchange Simulation with Incremental Coarsening. <i>Journal of Chemical Theory and Computation</i> , 2006 , 2, 656-66	6.4	64
83	Steady-state simulations using weighted ensemble path sampling. <i>Journal of Chemical Physics</i> , 2010 , 133, 014110	3.9	62
82	Simultaneous Computation of Dynamical and Equilibrium Information Using a Weighted Ensemble of Trajectories. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 2658-2667	6.4	60
81	Statistical Physics of Biomolecules		59
80	Overcoming finite-sampling errors in fast-switching free-energy estimates: extrapolative analysis of a molecular system. <i>Chemical Physics Letters</i> , 2002 , 351, 445-453	2.5	58
79	Structure of native lens connexin 46/50 intercellular channels by cryo-EM. <i>Nature</i> , 2018 , 564, 372-377	50.4	52
78	Efficient Atomistic Simulation of Pathways and Calculation of Rate Constants for a Protein-Peptide Binding Process: Application to the MDM2 Protein and an Intrinsically Disordered p53 Peptide. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 3440-5	6.4	51
77	Best Practices for Quantification of Uncertainty and Sampling Quality in Molecular Simulations [Article v1.0]. <i>Living Journal of Computational Molecular Science</i> , 2018 , 1,	10.1	51
76	Efficient dynamic importance sampling of rare events in one dimension. <i>Physical Review E</i> , 2001 , 63, 016702	10.2	50
75	On the structural convergence of biomolecular simulations by determination of the effective sample size. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 12876-82	3.4	49
74	Transition events in butane simulations: Similarities across models. <i>Journal of Chemical Physics</i> , 2002 , 116, 2586-2591	3.9	49
73	Best Practices for Foundations in Molecular Simulations [Article v1.0]. <i>Living Journal of Computational Molecular Science</i> , 2019 , 1,	10.1	49
72	Simulations of the alternating access mechanism of the sodium symporter Mhp1. <i>Biophysical Journal</i> , 2011 , 101, 2399-407	2.9	47
71	Accurate Estimation of Protein Folding and Unfolding Times: Beyond Markov State Models. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 3473-81	6.4	45
70	Statistical mechanics of membrane adhesion by reversible molecular bonds. <i>Physical Review Letters</i> , 1995 , 74, 3900-3903	7.4	45
69	Path-sampling strategies for simulating rare events in biomolecular systems. <i>Current Opinion in Structural Biology</i> , 2017 , 43, 88-94	8.1	44
68	Systematic Finite-Sampling Inaccuracy in Free Energy Differences and Other Nonlinear Quantities. <i>Journal of Statistical Physics</i> , 2004 , 114, 1303-1323	1.5	40
67	Critique of primitive model electrolyte theories. <i>Physical Review E</i> , 1997 , 56, 6569-6580	2.4	38

66	Beyond microscopic reversibility: Are observable non-equilibrium processes precisely reversible?. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 2520-2527	6.4	33
65	Heterogeneous path ensembles for conformational transitions in semi-atomistic models of adenylate kinase. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 3527-3539	6.4	31
64	Asymmetric primitive-model electrolytes: Debye-Hückel theory, criticality, and energy bounds. <i>Physical Review E</i> , 2001 , 64, 011206	2.4	31
63	Escape of a Small Molecule from Inside T4 Lysozyme by Multiple Pathways. <i>Biophysical Journal</i> , 2018 , 114, 1058-1066	2.9	30
62	Simple estimation of absolute free energies for biomolecules. <i>Journal of Chemical Physics</i> , 2006 , 124, 104105	3.9	30
61	Efficient stochastic simulation of chemical kinetics networks using a weighted ensemble of trajectories. <i>Journal of Chemical Physics</i> , 2013 , 139, 115105	3.9	29
60	Automated sampling assessment for molecular simulations using the effective sample size. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 3048-3057	6.4	28
59	Connexin-46/50 in a dynamic lipid environment resolved by CryoEM at 1.9 Å. <i>Nature Communications</i> , 2020 , 11, 4331	17.4	27
58	Vesicle-vesicle adhesion by mobile lock-and-key molecules: Debye-Hückel theory and Monte Carlo simulation. <i>Physical Review E</i> , 1998 , 57, 964-977	2.4	25
57	A Second Look at Canonical Sampling of Biomolecules Using Replica Exchange Simulation [J. Chem. Theory Comput. 2, 1200-1202 (2006)]. <i>Journal of Chemical Theory and Computation</i> , 2006 , 2, 1693	6.4	24
56	High-throughput, single-particle tracking reveals nested membrane domains that dictate KRas diffusion and trafficking. <i>ELife</i> , 2019 , 8,	8.9	23
55	Computational Estimation of Microsecond to Second Atomistic Folding Times. <i>Journal of the American Chemical Society</i> , 2019 , 141, 6519-6526	16.4	22
54	General library-based Monte Carlo technique enables equilibrium sampling of semi-atomistic protein models. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 10891-904	3.4	22
53	Unbiased Rare Event Sampling in Spatial Stochastic Systems Biology Models Using a Weighted Ensemble of Trajectories. <i>PLoS Computational Biology</i> , 2016 , 12, e1004611	5	22
52	Annealed importance sampling of peptides. <i>Journal of Chemical Physics</i> , 2007 , 127, 065101	3.9	20
51	Exact thermodynamic formulation of chemical association. <i>Journal of Chemical Physics</i> , 1998 , 109, 7961-7981	3.9	20
50	Estimating first-passage time distributions from weighted ensemble simulations and non-Markovian analyses. <i>Protein Science</i> , 2016 , 25, 67-78	6.3	20
49	Tools for channels: moving towards molecular calculations of gating and permeation in ion channel biophysics. <i>Journal of Molecular Graphics and Modelling</i> , 2004 , 22, 359-68	2.8	16

48	Statistical Uncertainty Analysis for Small-Sample, High Log-Variance Data: Cautions for Bootstrapping and Bayesian Bootstrapping. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 3499-3509	6.4	15
47	Biophysical comparison of ATP synthesis mechanisms shows a kinetic advantage for the rotary process. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016 , 113, 11220-11225	11.5	14
46	Peptide conformational equilibria computed via a single-stage shifting protocol. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 9096-103	3.4	14
45	Absolute Free energies estimated by combining precalculated molecular fragment libraries. <i>Journal of Computational Chemistry</i> , 2009 , 30, 1680-91	3.5	12
44	Supramolecular self assembly of nanodril-like structures for intracellular delivery. <i>Journal of Controlled Release</i> , 2018 , 282, 76-89	11.7	11
43	Tunable, mixed-resolution modeling using library-based Monte Carlo and graphics processing units. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 2921-2929	6.4	10
42	A black-box re-weighting analysis can correct flawed simulation data. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008 , 105, 7982-7	11.5	10
41	Molecular dynamics simulations of ionic concentration gradients across model bilayers. <i>Journal of Chemical Physics</i> , 2003 , 118, 1957-1969	3.9	9
40	#COVIDisAirborne: AI-Enabled Multiscale Computational Microscopy of Delta SARS-CoV-2 in a Respiratory Aerosol 2021 ,		9
39	A Suite of Tutorials for the WESTPA Rare-Events Sampling Software [Article v1.0]. <i>Living Journal of Computational Molecular Science</i> , 2019 , 1,	10.1	9
38	Vascular K channel structural dynamics reveal regulatory mechanism by Mg-nucleotides. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021 , 118,	11.5	9
37	What Markov State Models Can and Cannot Do: Correlation versus Path-Based Observables in Protein-Folding Models. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 3119-3133	6.4	9
36	Accelerating molecular Monte Carlo simulations using distance and orientation-dependent energy tables: tuning from atomistic accuracy to smoothed "coarse-grained" models. <i>Journal of Computational Chemistry</i> , 2012 , 33, 268-75	3.5	8
35	Extending fragment-based free energy calculations with library Monte Carlo simulation: annealing in interaction space. <i>Journal of Computational Chemistry</i> , 2011 , 32, 1135-43	3.5	8
34	Tunable Coarse Graining for Monte Carlo Simulations of Proteins via Smoothed Energy Tables: Direct and Exchange Simulations. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 5161-5177	6.4	7
33	Efficient equilibrium sampling of all-atom peptides using library-based Monte Carlo. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 5870-7	3.4	7
32	Resampling improves the efficiency of a "fast-switch" equilibrium sampling protocol. <i>Journal of Chemical Physics</i> , 2009 , 130, 081102	3.9	7
31	Middle-way flexible docking: Pose prediction using mixed-resolution Monte Carlo in estrogen receptor <i>PLoS ONE</i> , 2019 , 14, e0215694	3.7	6

30	A kinetic mechanism for enhanced selectivity of membrane transport. <i>PLoS Computational Biology</i> , 2020 , 16, e1007789	5	6
29	Tabulation as a high-resolution alternative to coarse-graining protein interactions: Initial application to virus capsid subunits. <i>Journal of Chemical Physics</i> , 2015 , 143, 243159	3.9	6
28	OPTIMIZING WEIGHTED ENSEMBLE SAMPLING OF STEADY STATES. <i>Multiscale Modeling and Simulation</i> , 2020 , 18, 646-673	1.8	6
27	Accelerated Estimation of Long-Timescale Kinetics from Weighted Ensemble Simulation via Non-Markovian "Microbin" Analysis. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 6763-6775	6.4	6
26	Structural integrity of the ribonuclease H domain in HIV-1 reverse transcriptase. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015 , 83, 1526-38	4.2	5
25	Chemical association via exact thermodynamic formulations. <i>Chemical Physics Letters</i> , 1998 , 293, 461-468.	5	5
24	EmrE reminds us to expect the unexpected in membrane transport. <i>Journal of General Physiology</i> , 2020 , 152,	3.4	5
23	Connexin 46 and connexin 50 gap junction channel properties are shaped by structural and dynamic features of their N-terminal domains. <i>Journal of Physiology</i> , 2021 , 599, 3313-3335	3.9	5
22	Entire-Dataset Analysis of NMR Fast-Exchange Titration Spectra: A Mg Titration Analysis for HIV-1 Ribonuclease H Domain. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 12420-12431	3.4	5
21	A systems-biology approach to molecular machines: Exploration of alternative transporter mechanisms. <i>PLoS Computational Biology</i> , 2020 , 16, e1007884	5	4
20	Rapid sampling of all-atom peptides using a library-based polymer-growth approach. <i>Journal of Computational Chemistry</i> , 2011 , 32, 396-405	3.5	4
19	Absolute free energies and equilibrium ensembles of dense fluids computed from a nondynamic growth method. <i>Journal of Chemical Physics</i> , 2009 , 131, 214110	3.9	4
18	Demonstrated Convergence of the Equilibrium Ensemble for a Fast United-Residue Protein Model. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 1860-6	6.4	4
17	Should Virus Capsids Assemble Perfectly? Theory and Observation of Defects. <i>Biophysical Journal</i> , 2020 , 119, 1781-1790	2.9	3
16	Transient probability currents provide upper and lower bounds on non-equilibrium steady-state currents in the Smoluchowski picture. <i>Journal of Chemical Physics</i> , 2019 , 151, 174108	3.9	3
15	Biophysical comparison of ATP-driven proton pumping mechanisms suggests a kinetic advantage for the rotary process depending on coupling ratio. <i>PLoS ONE</i> , 2017 , 12, e0173500	3.7	3
14	Key biology you should have learned in physics class: Using ideal-gas mixtures to understand biomolecular machines. <i>American Journal of Physics</i> , 2020 , 88, 182-193	0.7	2
13	Preface: Special Topic on Enhanced Sampling for Molecular Systems. <i>Journal of Chemical Physics</i> , 2018 , 149, 072001	3.9	2

12	Connexin-46/50 in a dynamic lipid environment resolved by CryoEM at 1.9 Å		2
11	A gentle introduction to the non-equilibrium physics of trajectories: Theory, algorithms, and biomolecular applications.. <i>American Journal of Physics</i> , 2021 , 89, 1048-1061	0.7	2
10	Why We Need the Living Journal of Computational Molecular Science. <i>Living Journal of Computational Molecular Science</i> , 2019 , 1,	10.1	2
9	Computational estimation of ms-sec atomistic folding times		2
8	What Markov state models can and cannot do: Correlation versus path-based observables in protein folding models		2
7	Systematic Testing of Belief-Propagation Estimates for Absolute Free Energies in Atomistic Peptides and Proteins. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 426-443	6.4	1
6	Extensive Evaluation of Weighted Ensemble Strategies for Calculating Rate Constants and Binding Affinities of Molecular Association/Dissociation Processes		1
5	Principles and Practicalities of Canonical Mixed-Resolution Sampling of Biomolecules 2008 , 171-184		1
4	Probing Membrane Nanodomain Organization with Single Particle Tracking via Photoactivated Localization Microscopy (spt-PALM). <i>Microscopy and Microanalysis</i> , 2019 , 25, 1248-1249	0.5	0
3	Continuum dynamics and statistical correction of compositional heterogeneity in multivalent IDP oligomers resolved by single-particle EM.. <i>Journal of Molecular Biology</i> , 2022 , 167520	6.5	0
2	Visualization of Protein-Lipid Interactions in Connexin-46/50 Intercellular Communication Channels at 2.1 Å Resolution. <i>Microscopy and Microanalysis</i> , 2019 , 25, 1216-1217	0.5	
1	Critique of Electrolyte Theories Using Thermodynamic Bounds 2002 , 415-418		