Daniel M Zuckerman

List of Publications by Year in Descending Order

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	Continuum dynamics and statistical correction of compositional heterogeneity in multivalent IDP oligomers resolved by single-particle EM.. *Journal of Molecular Biology*, **2022**, 167520	6.5	0
100	A gentle introduction to the non-equilibrium physics of trajectories: Theory, algorithms, and biomolecular applications.. *American Journal of Physics*, **2021**, 89, 1048-1061	0.7	2
99	#COVIDisAirborne: AI-Enabled Multiscale Computational Microscopy of Delta SARS-CoV-2 in a Respiratory Aerosol **2021**,		9
98	Vascular K channel structural dynamics reveal regulatory mechanism by Mg-nucleotides. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	9
97	What Markov State Models Can and Cannot Do: Correlation versus Path-Based Observables in Protein-Folding Models. *Journal of Chemical Theory and Computation*, **2021**, 17, 3119-3133	6.4	9
96	Connexin 46 and connexin 50 gap junction channel properties are shaped by structural and dynamic features of their N-terminal domains. *Journal of Physiology*, **2021**, 599, 3313-3335	3.9	5
95	Should Virus Capsids Assemble Perfectly? Theory and Observation of Defects. *Biophysical Journal*, **2020**, 119, 1781-1790	2.9	3
94	A systems-biology approach to molecular machines: Exploration of alternative transporter mechanisms. *PLoS Computational Biology*, **2020**, 16, e1007884	5	4
93	A kinetic mechanism for enhanced selectivity of membrane transport. *PLoS Computational Biology*, **2020**, 16, e1007789	5	6
92	Key biology you should have learned in physics class: Using ideal-gas mixtures to understand biomolecular machines. *American Journal of Physics*, **2020**, 88, 182-193	0.7	2
91	OPTIMIZING WEIGHTED ENSEMBLE SAMPLING OF STEADY STATES. *Multiscale Modeling and Simulation*, **2020**, 18, 646-673	1.8	6
90	EmrE reminds us to expect the unexpected in membrane transport. *Journal of General Physiology*, **2020**, 152,	3.4	5
89	Accelerated Estimation of Long-Timescale Kinetics from Weighted Ensemble Simulation via Non-Markovian "Microbin" Analysis. *Journal of Chemical Theory and Computation*, **2020**, 16, 6763-6775	6.4	6
88	Connexin-46/50 in a dynamic lipid environment resolved by CryoEM at 1.9 Å *Nature Communications*, **2020**, 11, 4331	17.4	27
87	Middle-way flexible docking: Pose prediction using mixed-resolution Monte Carlo in estrogen receptor α *PLoS ONE*, **2019**, 14, e0215694	3.7	6
86	Statistical Uncertainty Analysis for Small-Sample, High Log-Variance Data: Cautions for Bootstrapping and Bayesian Bootstrapping. *Journal of Chemical Theory and Computation*, **2019**, 15, 3499-3509	6.4	15
85	Computational Estimation of Microsecond to Second Atomistic Folding Times. *Journal of the American Chemical Society*, **2019**, 141, 6519-6526	16.4	22

84	Probing Membrane Nanodomain Organization with Single Particle Tracking via Photoactivated Localization Microscopy (spt-PALM). *Microscopy and Microanalysis*, **2019**, 25, 1248-1249	0.5	0
83	Visualization of Protein-Lipid Interactions in Connexin-46/50 Intercellular Communication Channels at 2.1 Resolution. *Microscopy and Microanalysis*, **2019**, 25, 1216-1217	0.5	
82	Transient probability currents provide upper and lower bounds on non-equilibrium steady-state currents in the Smoluchowski picture. *Journal of Chemical Physics*, **2019**, 151, 174108	3.9	3
81	Why We Need the Living Journal of Computational Molecular Science. *Living Journal of Computational Molecular Science*, **2019**, 1,	10.1	2
80	Best Practices for Foundations in Molecular Simulations [Article v1.0]. *Living Journal of Computational Molecular Science*, **2019**, 1,	10.1	49
79	A Suite of Tutorials for the WESTPA Rare-Events Sampling Software [Article v1.0]. *Living Journal of Computational Molecular Science*, **2019**, 1,	10.1	9
78	High-throughput, single-particle tracking reveals nested membrane domains that dictate KRas diffusion and trafficking. *ELife*, **2019**, 8,	8.9	23
77	Supramolecular self assembly of nanodrill-like structures for intracellular delivery. *Journal of Controlled Release*, **2018**, 282, 76-89	11.7	11
76	Systematic Testing of Belief-Propagation Estimates for Absolute Free Energies in Atomistic Peptides and Proteins. *Journal of Chemical Theory and Computation*, **2018**, 14, 426-443	6.4	1
75	Escape of a Small Molecule from Inside T4Lysozyme by Multiple Pathways. *Biophysical Journal*, **2018**, 114, 1058-1066	2.9	30
74	Preface: Special Topic on Enhanced Sampling for Molecular Systems. *Journal of Chemical Physics*, **2018**, 149, 072001	3.9	2
73	Best Practices for Quantification of Uncertainty and Sampling Quality in Molecular Simulations [Article v1.0]. *Living Journal of Computational Molecular Science*, **2018**, 1,	10.1	51
72	Structure of native lens connexin 46/50 intercellular channels by cryo-EM. *Nature*, **2018**, 564, 372-377	50.4	52
71	Weighted Ensemble Simulation: Review of Methodology, Applications, and Software. *Annual Review of Biophysics*, **2017**, 46, 43-57	21.1	101
70	Path-sampling strategies for simulating rare events in biomolecular systems. *Current Opinion in Structural Biology*, **2017**, 43, 88-94	8.1	44
69	Biophysical comparison of ATP-driven proton pumping mechanisms suggests a kinetic advantage for the rotary process depending on coupling ratio. *PLoS ONE*, **2017**, 12, e0173500	3.7	3
68	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. *Journal of Physical Chemistry Letters*, **2016**, 7, 3440-5	6.4	51
67	Biophysical comparison of ATP synthesis mechanisms shows a kinetic advantage for the rotary process. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 11220-11225	11.5	14

66	Accurate Estimation of Protein Folding and Unfolding Times: Beyond Markov State Models. *Journal of Chemical Theory and Computation*, **2016**, 12, 3473-81	6.4	45
65	Unbiased Rare Event Sampling in Spatial Stochastic Systems Biology Models Using a Weighted Ensemble of Trajectories. *PLoS Computational Biology*, **2016**, 12, e1004611	5	22
64	Entire-Dataset Analysis of NMR Fast-Exchange Titration Spectra: A Mg Titration Analysis for HIV-1 Ribonuclease H Domain. *Journal of Physical Chemistry B*, **2016**, 120, 12420-12431	3.4	5
63	Estimating first-passage time distributions from weighted ensemble simulations and non-Markovian analyses. *Protein Science*, **2016**, 25, 67-78	6.3	20
62	Tabulation as a high-resolution alternative to coarse-graining protein interactions: Initial application to virus capsid subunits. *Journal of Chemical Physics*, **2015**, 143, 243159	3.9	6
61	Structural integrity of the ribonuclease H domain in HIV-1 reverse transcriptase. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 1526-38	4.2	5
60	WESTPA: an interoperable, highly scalable software package for weighted ensemble simulation and analysis. *Journal of Chemical Theory and Computation*, **2015**, 11, 800-9	6.4	75
59	Tunable Coarse Graining for Monte Carlo Simulations of Proteins via Smoothed Energy Tables: Direct and Exchange Simulations. *Journal of Chemical Theory and Computation*, **2014**, 10, 5161-5177	6.4	7
58	Simultaneous Computation of Dynamical and Equilibrium Information Using a Weighted Ensemble of Trajectories. *Journal of Chemical Theory and Computation*, **2014**, 10, 2658-2667	6.4	60
57	Efficient stochastic simulation of chemical kinetics networks using a weighted ensemble of trajectories. *Journal of Chemical Physics*, **2013**, 139, 115105	3.9	29
56	Accelerating molecular Monte Carlo simulations using distance and orientation-dependent energy tables: tuning from atomistic accuracy to smoothed "coarse-grained" models. *Journal of Computational Chemistry*, **2012**, 33, 268-75	3.5	8
55	Tunable, mixed-resolution modeling using library-based Monte Carlo and graphics processing units. *Journal of Chemical Theory and Computation*, **2012**, 8, 2921-2929	6.4	10
54	Simulations of the alternating access mechanism of the sodium symporter Mhp1. *Biophysical Journal*, **2011**, 101, 2399-407	2.9	47
53	Equilibrium sampling in biomolecular simulations. *Annual Review of Biophysics*, **2011**, 40, 41-62	21.1	171
52	Rapid sampling of all-atom peptides using a library-based polymer-growth approach. *Journal of Computational Chemistry*, **2011**, 32, 396-405	3.5	4
51	Extending fragment-based free energy calculations with library Monte Carlo simulation: annealing in interaction space. *Journal of Computational Chemistry*, **2011**, 32, 1135-43	3.5	8
50	Beyond microscopic reversibility: Are observable non-equilibrium processes precisely reversible?. *Journal of Chemical Theory and Computation*, **2011**, 7, 2520-2527	6.4	33
49	The "weighted ensemble" path sampling method is statistically exact for a broad class of stochastic processes and binning procedures. *Journal of Chemical Physics*, **2010**, 132, 054107	3.9	122

48	Steady-state simulations using weighted ensemble path sampling. *Journal of Chemical Physics*, **2010**, 133, 014110	3.9	62
47	Efficient equilibrium sampling of all-atom peptides using library-based Monte Carlo. *Journal of Physical Chemistry B*, **2010**, 114, 5870-7	3.4	7
46	Heterogeneous path ensembles for conformational transitions in semi-atomistic models of adenylate kinase. *Journal of Chemical Theory and Computation*, **2010**, 6, 3527-3539	6.4	31
45	Automated sampling assessment for molecular simulations using the effective sample size. *Journal of Chemical Theory and Computation*, **2010**, 6, 3048-3057	6.4	28
44	Absolute free energies and equilibrium ensembles of dense fluids computed from a nondynamic growth method. *Journal of Chemical Physics*, **2009**, 131, 214110	3.9	4
43	Resampling improves the efficiency of a "fast-switch" equilibrium sampling protocol. *Journal of Chemical Physics*, **2009**, 130, 081102	3.9	7
42	Absolute free energies estimated by combining precalculated molecular fragment libraries. *Journal of Computational Chemistry*, **2009**, 30, 1680-91	3.5	12
41	General library-based Monte Carlo technique enables equilibrium sampling of semi-atomistic protein models. *Journal of Physical Chemistry B*, **2009**, 113, 10891-904	3.4	22
40	Quantifying uncertainty and sampling quality in biomolecular simulations. *Annual Reports in Computational Chemistry*, **2009**, 5, 23-48	1.8	216
39	A black-box re-weighting analysis can correct flawed simulation data. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 7982-7	11.5	10
38	Principles and Practicalities of Canonical Mixed-Resolution Sampling of Biomolecules **2008**, 171-184		1
37	On the structural convergence of biomolecular simulations by determination of the effective sample size. *Journal of Physical Chemistry B*, **2007**, 111, 12876-82	3.4	49
36	Demonstrated Convergence of the Equilibrium Ensemble for a Fast United-Residue Protein Model. *Journal of Chemical Theory and Computation*, **2007**, 3, 1860-6	6.4	4
35	Transition-event durations in one-dimensional activated processes. *Journal of Chemical Physics*, **2007**, 126, 074504	3.9	79
34	Efficient and verified simulation of a path ensemble for conformational change in a united-residue model of calmodulin. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 18043-8	11.5	101
33	Annealed importance sampling of peptides. *Journal of Chemical Physics*, **2007**, 127, 065101	3.9	20
32	Simple estimation of absolute free energies for biomolecules. *Journal of Chemical Physics*, **2006**, 124, 104105	3.9	30
31	Resolution exchange simulation. *Physical Review Letters*, **2006**, 96, 028105	7.4	167

30	Ensemble-based convergence analysis of biomolecular trajectories. *Biophysical Journal*, **2006**, 91, 164-72	2.9	95
29	Resolution Exchange Simulation with Incremental Coarsening. *Journal of Chemical Theory and Computation*, **2006**, 2, 656-66	6.4	64
28	A Second Look at Canonical Sampling of Biomolecules using Replica Exchange Simulation. *Journal of Chemical Theory and Computation*, **2006**, 2, 12001202	6.4	84
27	A Second Look at Canonical Sampling of Biomolecules Using Replica Exchange Simulation [J. Chem. Theory Comput. 2, 1200-1202 (2006)]. *Journal of Chemical Theory and Computation*, **2006**, 2, 1693	6.4	24
26	Comparison of free energy methods for molecular systems. *Journal of Chemical Physics*, **2006**, 125, 184114	3.9	115
25	Peptide conformational equilibria computed via a single-stage shifting protocol. *Journal of Physical Chemistry B*, **2005**, 109, 9096-103	3.4	14
24	Single-ensemble nonequilibrium path-sampling estimates of free energy differences. *Journal of Chemical Physics*, **2004**, 120, 10876-9	3.9	94
23	Systematic Finite-Sampling Inaccuracy in Free Energy Differences and Other Nonlinear Quantities. *Journal of Statistical Physics*, **2004**, 114, 1303-1323	1.5	40
22	Efficient use of nonequilibrium measurement to estimate free energy differences for molecular systems. *Journal of Computational Chemistry*, **2004**, 25, 1749-59	3.5	67
21	Tools for channels: moving towards molecular calculations of gating and permeation in ion channel biophysics. *Journal of Molecular Graphics and Modelling*, **2004**, 22, 359-68	2.8	16
20	Simulation of an Ensemble of Conformational Transitions in a United-Residue Model of Calmodulin. *Journal of Physical Chemistry B*, **2004**, 108, 5127-5137	3.4	77
19	Molecular dynamics simulations of ionic concentration gradients across model bilayers. *Journal of Chemical Physics*, **2003**, 118, 1957-1969	3.9	9
18	Critique of Electrolyte Theories Using Thermodynamic Bounds **2002**, 415-418		
17	Overcoming finite-sampling errors in fast-switching free-energy estimates: extrapolative analysis of a molecular system. *Chemical Physics Letters*, **2002**, 351, 445-453	2.5	58
16	Theory of a systematic computational error in free energy differences. *Physical Review Letters*, **2002**, 89, 180602	7.4	130
15	Transition events in butane simulations: Similarities across models. *Journal of Chemical Physics*, **2002**, 116, 2586-2591	3.9	49
14	Hydrophobic Matching Mechanism Investigated by Molecular Dynamics Simulations. *Langmuir*, **2002**, 18, 1340-1351	4	79
13	Efficient dynamic importance sampling of rare events in one dimension. *Physical Review E*, **2001**, 63, 016702	2.4	50

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12	Asymmetric primitive-model electrolytes: Debye-H□kel theory, criticality, and energy bounds. *Physical Review E*, **2001**, 64, 011206	2.4	31
11	Dynamic reaction paths and rates through importance-sampled stochastic dynamics. *Journal of Chemical Physics*, **1999**, 111, 9475-9484	3.9	78
10	Chemical association via exact thermodynamic formulations. *Chemical Physics Letters*, **1998**, 293, 461-468	2.5	5
9	Vesicle-vesicle adhesion by mobile lock-and-key molecules: Debye-H□kel theory and Monte Carlo simulation. *Physical Review E*, **1998**, 57, 964-977	2.4	25
8	Exact thermodynamic formulation of chemical association. *Journal of Chemical Physics*, **1998**, 109, 7961-7981	3.9	20
7	Critique of primitive model electrolyte theories. *Physical Review E*, **1997**, 56, 6569-6580	2.4	38
6	Statistical mechanics of membrane adhesion by reversible molecular bonds. *Physical Review Letters*, **1995**, 74, 3900-3903	7.4	45
5	Statistical Physics of Biomolecules		59
4	Connexin-46/50 in a dynamic lipid environment resolved by CryoEM at 1.9 □		2
3	Computational estimation of ms-sec atomistic folding times		2
2	Extensive Evaluation of Weighted Ensemble Strategies for Calculating Rate Constants and Binding Affinities of Molecular Association/Dissociation Processes		1
1	What Markov state models can and cannot do: Correlation versus path-based observables in protein folding models		2