Michael R Shirts

List of Publications by Year in Descending Order

90 papers	12,126 citations	39 h-index	110 g-index
116 ext. papers	13,890 ext. citations	4.9 avg, IF	6.5 L-index

#	Paper	IF	Citations
90	physical_validation: A Python package to assess the physical validity of molecular simulation results. *Journal of Open Source Software*, **2022**, 7, 3981	5.2	
89	Potential Foldamers Based on an Terphenyl Amino Acid. *Organic Letters*, **2021**, 23, 4855-4859	6.2	2
88	Development and Benchmarking of Open Force Field v1.0.0-the Parsley Small-Molecule Force Field. *Journal of Chemical Theory and Computation*, **2021**, 17, 6262-6280	6.4	12
87	Using a Coarse-Grained Modeling Framework to Identify Oligomeric Motifs with Tunable Secondary Structure. *Journal of Chemical Theory and Computation*, **2021**, 17, 6018-6035	6.4	0
86	Expanded Ensemble Methods Can be Used to Accurately Predict Protein-Ligand Relative Binding Free Energies. *Journal of Chemical Theory and Computation*, **2021**, 17, 6536-6547	6.4	1
85	A nanostructured bifunctional acidBase catalyst resin formed by lyotropic liquid crystal monomers. *Canadian Journal of Chemistry*, **2020**, 98, 332-336	0.9	2
84	Statistically Optimal Continuous Free Energy Surfaces from Biased Simulations and Multistate Reweighting. *Journal of Chemical Theory and Computation*, **2020**, 16, 4107-4125	6.4	3
83	The SAMPL6 SAMPLing challenge: assessing the reliability and efficiency of binding free energy calculations. *Journal of Computer-Aided Molecular Design*, **2020**, 34, 601-633	4.2	55
82	Adaptive Ensemble Biomolecular Applications at Scale. *SN Computer Science*, **2020**, 1, 1	2	2
81	Best Practices for Alchemical Free Energy Calculations [Article v1.0]. *Living Journal of Computational Molecular Science*, **2020**, 2,	10.1	38
80	Statistical Mechanical Approximations to More Efficiently Determine Polymorph Free Energy Differences for Small Organic Molecules. *Journal of Chemical Theory and Computation*, **2020**, 16, 6503-6512	6.4	3
79	Statistical Inference of Transport Mechanisms and Long Time Scale Behavior from Time Series of Solute Trajectories in Nanostructured Membranes. *Journal of Physical Chemistry B*, **2020**, 124, 8110-8123	3.4	5
78	Capturing Subdiffusive Solute Dynamics and Predicting Selectivity in Nanoscale Pores with Time Series Modeling. *Journal of Chemical Theory and Computation*, **2020**, 16, 5456-5473	6.4	2
77	Configurational mapping significantly increases the efficiency of solid-solid phase coexistence calculations via molecular dynamics: Determining the FCC-HCP coexistence line of Lennard-Jones particles. *Journal of Chemical Physics*, **2019**, 150, 164112	3.9	0
76	Histogram-Free Reweighting with Grand Canonical Monte Carlo: Post-simulation Optimization of Non-bonded Potentials for Phase Equilibria. *Journal of Chemical & Engineering Data*, **2019**, 64, 3701-3717	2.8	3
75	Exploring the Multi-minima Behavior of Small Molecule Crystal Polymorphs at Finite Temperature. *Crystal Growth and Design*, **2019**, 19, 5568-5580	3.5	16
74	Chemically Selective Transport in a Cross-Linked H Phase Lyotropic Liquid Crystal Membrane. *Journal of Physical Chemistry B*, **2019**, 123, 6314-6330	3.4	5

73	Adding Anisotropy to the Standard Quasi-Harmonic Approximation Still Fails in Several Ways to Capture Organic Crystal Thermodynamics. *Crystal Growth and Design*, **2019**, 19, 6911-6924	3.5	8
72	Why We Need the Living Journal of Computational Molecular Science. *Living Journal of Computational Molecular Science*, **2019**, 1,	10.1	2
71	Understanding the Nanoscale Structure of Inverted Hexagonal Phase Lyotropic Liquid Crystal Polymer Membranes. *Journal of Physical Chemistry B*, **2019**, 123, 289-309	3.4	8
70	Toward Learned Chemical Perception of Force Field Typing Rules. *Journal of Chemical Theory and Computation*, **2019**, 15, 402-423	6.4	23
69	Using reweighting and free energy surface interpolation to predict solid-solid phase diagrams. *Journal of Chemical Physics*, **2018**, 148, 144104	3.9	12
68	Configuration-Sampling-Based Surrogate Models for Rapid Parameterization of Non-Bonded Interactions. *Journal of Chemical Theory and Computation*, **2018**, 14, 3144-3162	6.4	18
67	Uncertainty quantification confirms unreliable extrapolation toward high pressures for united-atom Mie -6 force field. *Journal of Chemical Physics*, **2018**, 149, 114109	3.9	7
66	Escaping Atom Types in Force Fields Using Direct Chemical Perception. *Journal of Chemical Theory and Computation*, **2018**, 14, 6076-6092	6.4	62
65	Thermal Gradient Approach for the Quasi-harmonic Approximation and Its Application to Improved Treatment of Anisotropic Expansion. *Journal of Chemical Theory and Computation*, **2018**, 14, 5904-5919	6.4	9
64	Testing for physical validity in molecular simulations. *PLoS ONE*, **2018**, 13, e0202764	3.7	22
63	Capturing Entropic Contributions to Temperature-Mediated Polymorphic Transformations Through Molecular Modeling. *Crystal Growth and Design*, **2017**, 17, 1775-1787	3.5	34
62	Approaches for calculating solvation free energies and enthalpies demonstrated with an update of the FreeSolv database. *Journal of Chemical & Engineering Data*, **2017**, 62, 1559-1569	2.8	114
61	Effects of protein properties on adsorption and transport in polymer-grafted ion exchangers: A multiscale modeling study. *AICHE Journal*, **2017**, 63, 4564-4575	3.6	10
60	Overview of the SAMPL5 host-guest challenge: Are we doing better?. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 1-19	4.2	116
59	Lessons learned from comparing molecular dynamics engines on the SAMPL5 dataset. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 147-161	4.2	81
58	Effects of a More Accurate Polarizable Hamiltonian on Polymorph Free Energies Computed Efficiently by Reweighting Point-Charge Potentials. *Journal of Chemical Theory and Computation*, **2016**, 12, 3491-505	6.4	19
57	Rapid Computation of Thermodynamic Properties over Multidimensional Nonbonded Parameter Spaces Using Adaptive Multistate Reweighting. *Journal of Chemical Theory and Computation*, **2016**, 12, 1806-23	6.4	10
56	Comparison of Methods To Reweight from Classical Molecular Simulations to QM/MM Potentials. *Journal of Chemical Theory and Computation*, **2016**, 12, 1466-80	6.4	36

55	Blind prediction of cyclohexane-water distribution coefficients from the SAMPL5 challenge. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 927-944	4.2	80
54	Identifying Differences and Similarities in Static and Dynamic Contact Angles between Nanoscale and Microscale Textured Surfaces Using Molecular Dynamics Simulations. *Langmuir*, **2015**, 31, 7980-90	4	3
53	Linear basis function approach to efficient alchemical free energy calculations. 2. Inserting and deleting particles with coulombic interactions. *Journal of Chemical Theory and Computation*, **2015**, 11, 2536-49	6.4	39
52	Guidelines for the analysis of free energy calculations. *Journal of Computer-Aided Molecular Design*, **2015**, 29, 397-411	4.2	281
51	Effects of polymer graft properties on protein adsorption and transport in ion exchange chromatography: a multiscale modeling study. *Langmuir*, **2015**, 31, 4176-87	4	15
50	Converging free energies of binding in cucurbit[7]uril and octa-acid host-guest systems from SAMPL4 using expanded ensemble simulations. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 401-15	4.2	30
49	Multiscale modeling of protein adsorption and transport in macroporous and polymer-grafted ion exchangers. *AICHE Journal*, **2014**, 60, 3888-3901	3.6	19
48	Linear Basis Function Approach to Efficient Alchemical Free Energy Calculations. 1. Removal of Uncharged Atomic Sites. *Journal of Chemical Theory and Computation*, **2014**, 10, 1128-49	6.4	30
47	Thermodynamics of coupled protein adsorption and stability using hybrid Monte Carlo simulations. *Langmuir*, **2014**, 30, 4952-61	4	7
46	Investigating the mutation resistance of nonnucleoside inhibitors of HIV-RT using multiple microsecond atomistic simulations. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 130-44	4.2	5
45	Identifying ligand binding sites and poses using GPU-accelerated Hamiltonian replica exchange molecular dynamics. *Journal of Computer-Aided Molecular Design*, **2013**, 27, 989-1007	4.2	86
44	Simple Quantitative Tests to Validate Sampling from Thermodynamic Ensembles. *Journal of Chemical Theory and Computation*, **2013**, 9, 909-26	6.4	52
43	OpenMM 4: A Reusable, Extensible, Hardware Independent Library for High Performance Molecular Simulation. *Journal of Chemical Theory and Computation*, **2013**, 9, 461-469	6.4	440
42	GROMACS 4.5: a high-throughput and highly parallel open source molecular simulation toolkit. *Bioinformatics*, **2013**, 29, 845-54	7.2	4786
41	An introduction to best practices in free energy calculations. *Methods in Molecular Biology*, **2013**, 924, 271-311	1.4	72
40	Effects of Temperature Control Algorithms on Transport Properties and Kinetics in Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2013**, 9, 2887-99	6.4	213
39	Glycoside hydrolase processivity is directly related to oligosaccharide binding free energy. *Journal of the American Chemical Society*, **2013**, 135, 18831-9	16.4	71
38	Using Multistate Reweighting to Rapidly and Efficiently Explore Molecular Simulation Parameters Space for Nonbonded Interactions. *Journal of Chemical Theory and Computation*, **2013**, 9, 4700-17	6.4	13

37	Multistate reweighting and configuration mapping together accelerate the efficiency of thermodynamic calculations as a function of molecular geometry by orders of magnitude. *Journal of Chemical Physics*, **2013**, 138, 154108	3.9	9
36	Distinct aggregation mechanisms of monoclonal antibody under thermal and freeze-thaw stresses revealed by hydrogen exchange. *Pharmaceutical Research*, **2012**, 29, 236-50	4.5	120
35	Configurational preferences of arylamide helix mimetics via alchemical free energy calculations of relative binding affinities. *Journal of Physical Chemistry B*, **2012**, 116, 10856-69	3.4	5
34	Optimal pairwise and non-pairwise alchemical pathways for free energy calculations of molecular transformation in solution phase. *Journal of Chemical Physics*, **2012**, 136, 124120	3.9	36
33	Product binding varies dramatically between processive and nonprocessive cellulase enzymes. *Journal of Biological Chemistry*, **2012**, 287, 24807-13	5.4	49
32	Modeling of arylamide helix mimetics in the p53 peptide binding site of hDM2 suggests parallel and anti-parallel conformations are both stable. *PLoS ONE*, **2012**, 7, e43253	3.7	13
31	Best practices in free energy calculations for drug design. *Methods in Molecular Biology*, **2012**, 819, 425-67	1.4	28
30	Identifying low variance pathways for free energy calculations of molecular transformations in solution phase. *Journal of Chemical Physics*, **2011**, 135, 034114	3.9	61
29	A Benchmark Test Set for Alchemical Free Energy Transformations and Its Use to Quantify Error in Common Free Energy Methods. *Journal of Chemical Theory and Computation*, **2011**, 7, 4115-34	6.4	99
28	Alchemical free energy methods for drug discovery: progress and challenges. *Current Opinion in Structural Biology*, **2011**, 21, 150-60	8.1	382
27	Replica exchange and expanded ensemble simulations as Gibbs sampling: simple improvements for enhanced mixing. *Journal of Chemical Physics*, **2011**, 135, 194110	3.9	118
26	Probing carbohydrate product expulsion from a processive cellulase with multiple absolute binding free energy methods. *Journal of Biological Chemistry*, **2011**, 286, 18161-9	5.4	64
25	Dynamical reweighting: improved estimates of dynamical properties from simulations at multiple temperatures. *Journal of Chemical Physics*, **2011**, 134, 244107	3.9	50
24	Small molecule hydration free energies in explicit solvent: An extensive test of fixed-charge atomistic simulations. *Journal of Chemical Theory and Computation*, **2009**, 5, 350-358	6.4	279
23	Statistically optimal analysis of samples from multiple equilibrium states. *Journal of Chemical Physics*, **2008**, 129, 124105	3.9	1012
22	Chapter 4 Alchemical Free Energy Calculations: Ready for Prime Time?. *Annual Reports in Computational Chemistry*, **2007**, 3, 41-59	1.8	156
21	Accurate and efficient corrections for missing dispersion interactions in molecular simulations. *Journal of Physical Chemistry B*, **2007**, 111, 13052-63	3.4	141
20	Improved Methods for Side Chain and Loop Predictions via the Protein Local Optimization Program: Variable Dielectric Model for Implicitly Improving the Treatment of Polarization Effects. *Journal of Chemical Theory and Computation*, **2007**, 3, 2108-19	6.4	89

19	Multiscale Optimization of a Truncated Newton Minimization Algorithm and Application to Proteins and Protein-Ligand Complexes. *Journal of Chemical Theory and Computation*, **2007**, 3, 640-8	6.4	27
18	Parallelized-over-parts computation of absolute binding free energy with docking and molecular dynamics. *Journal of Chemical Physics*, **2006**, 125, 084901	3.9	81
17	The solvation interface is a determining factor in peptide conformational preferences. *Journal of Molecular Biology*, **2006**, 356, 248-56	6.5	40
16	Comparison of efficiency and bias of free energies computed by exponential averaging, the Bennett acceptance ratio, and thermodynamic integration. *Journal of Chemical Physics*, **2005**, 122, 144107	3.9	288
15	Direct calculation of the binding free energies of FKBP ligands. *Journal of Chemical Physics*, **2005**, 123, 084108	3.9	165
14	Solvation free energies of amino acid side chain analogs for common molecular mechanics water models. *Journal of Chemical Physics*, **2005**, 122, 134508	3.9	329
13	Extremely precise free energy calculations of amino acid side chain analogs: Comparison of common molecular mechanics force fields for proteins. *Journal of Chemical Physics*, **2003**, 119, 5740-5761	3.9	544
12	Equilibrium free energies from nonequilibrium measurements using maximum-likelihood methods. *Physical Review Letters*, **2003**, 91, 140601	7.4	360
11	Deviations from the Boltzmann distribution in small microcanonical quantum systems: Two approximate one-particle energy distributions. *Journal of Chemical Physics*, **2002**, 117, 5564-5575	3.9	7
10	Native-like mean structure in the unfolded ensemble of small proteins. *Journal of Molecular Biology* , **2002**, 323, 153-64	6.5	164
9	Simulation of folding of a small alpha-helical protein in atomistic detail using worldwide-distributed computing. *Journal of Molecular Biology*, **2002**, 323, 927-37	6.5	245
8	Mathematical analysis of coupled parallel simulations. *Physical Review Letters*, **2001**, 86, 4983-7	7.4	87
7	Free-energy calculations in structure-based drug design61-86		58
6	Development and Benchmarking of Open Force Field v1.0.0, the Parsley Small Molecule Force Field		2
5	Development and Benchmarking of Open Force Field v1.0.0, the Parsley Small Molecule Force Field		3
4	Development and Benchmarking of Open Force Field v1.0.0, the Parsley Small Molecule Force Field		2
3	Lessons learned from comparing molecular dynamics engines on the SAMPL5 dataset		2
2	Open Force Field Consortium: Escaping atom types using direct chemical perception with SMIRNOFF v0.1		11

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