Michael R Shirts

List of Publications by Year
in descending order

89 papers	15,303 citations	71102 41 h-index	46799 89 g-index
116 all docs	116 docs citations	116 times ranked	16362 citing authors

#	Article	IF	Citations
1	physical_validation: A Python package to assess the physical validity of molecular simulation results. Journal of Open Source Software, 2022, 7, 3981.	4.6	0
2	Bayesian-Inference-Driven Model Parametrization and Model Selection for 2CLJQ Fluid Models. Journal of Chemical Information and Modeling, 2022, , .	5.4	6
3	Identifying signatures of proteolytic stability and monomeric propensity in O-glycosylated insulin using molecular simulation. Journal of Computer-Aided Molecular Design, 2022, 36, 313-328.	2.9	2
4	Improving Force Field Accuracy by Training against Condensed-Phase Mixture Properties. Journal of Chemical Theory and Computation, 2022, 18, 3577-3592.	5.3	9
5	Open Force Field Evaluator: An Automated, Efficient, and Scalable Framework for the Estimation of Physical Properties from Molecular Simulation. Journal of Chemical Theory and Computation, 2022, 18, 3566-3576.	5.3	19
6	Potential Foldamers Based on an ortho-Terphenyl Amino Acid. Organic Letters, 2021, 23, 4855-4859.	4.6	3
7	Development and Benchmarking of Open Force Field v1.0.0â€"the Parsley Small-Molecule Force Field. Journal of Chemical Theory and Computation, 2021, 17, 6262-6280.	5.3	80
8	Using a Coarse-Grained Modeling Framework to Identify Oligomeric Motifs with Tunable Secondary Structure. Journal of Chemical Theory and Computation, 2021, 17, 6018-6035.	5.3	3
9	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.	5.3	7
10	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.	5.3	10
11	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.	2.6	7
12	Capturing Subdiffusive Solute Dynamics and Predicting Selectivity in Nanoscale Pores with Time Series Modeling. Journal of Chemical Theory and Computation, 2020, 16, 5456-5473.	5.3	3
13	A nanostructured bifunctional acidâ€"base catalyst resin formed by lyotropic liquid crystal monomers. Canadian Journal of Chemistry, 2020, 98, 332-336.	1.1	4
14	Statistically Optimal Continuous Free Energy Surfaces from Biased Simulations and Multistate Reweighting. Journal of Chemical Theory and Computation, 2020, 16, 4107-4125.	5.3	8
15	The SAMPL6 SAMPLing challenge: assessing the reliability and efficiency of binding free energy calculations. Journal of Computer-Aided Molecular Design, 2020, 34, 601-633.	2.9	86
16	Adaptive Ensemble Biomolecular Applications at Scale. SN Computer Science, 2020, 1, 1.	3.6	14
17	Best Practices for Alchemical Free Energy Calculations [Article v1.0]. Living Journal of Computational Molecular Science, 2020, 2, .	6.4	125
18	Exploring the Multi-minima Behavior of Small Molecule Crystal Polymorphs at Finite Temperature. Crystal Growth and Design, 2019, 19, 5568-5580.	3.0	24

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19	Chemically Selective Transport in a Cross-Linked H_{II} Phase Lyotropic Liquid Crystal Membrane. Journal of Physical Chemistry B, 2019, 123, 6314-6330.	2.6	6
20	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.	3.0	17
21	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.	3.0	3
22	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.	1.9	5
23	Understanding the Nanoscale Structure of Inverted Hexagonal Phase Lyotropic Liquid Crystal Polymer Membranes. Journal of Physical Chemistry B, 2019, 123, 289-309.	2.6	11
24	Toward Learned Chemical Perception of Force Field Typing Rules. Journal of Chemical Theory and Computation, 2019, 15, 402-423.	5.3	30
25	Why We Need the Living Journal of Computational Molecular Science. Living Journal of Computational Molecular Science, 2019, 1, .	6.4	2
26	Best Practices for Alchemical Free Energy Calculations [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 2, .	6.4	3
27	Using reweighting and free energy surface interpolation to predict solid-solid phase diagrams. Journal of Chemical Physics, 2018, 148, 144104.	3.0	19
28	Configuration-Sampling-Based Surrogate Models for Rapid Parameterization of Non-Bonded Interactions. Journal of Chemical Theory and Computation, 2018, 14, 3144-3162.	5.3	26
29	Uncertainty quantification confirms unreliable extrapolation toward high pressures for united-atom Mie Î»-6 force field. Journal of Chemical Physics, 2018, 149, 114109.	3.0	9
30	Escaping Atom Types in Force Fields Using Direct Chemical Perception. Journal of Chemical Theory and Computation, 2018, 14, 6076-6092.	5.3	110
31	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.	5.3	13
32	Testing for physical validity in molecular simulations. PLoS ONE, 2018, 13, e0202764.	2.5	30
33	Capturing Entropic Contributions to Temperature-Mediated Polymorphic Transformations Through Molecular Modeling. Crystal Growth and Design, 2017, 17, 1775-1787.	3.0	43
34	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.	1.9	164
35	Effects of protein properties on adsorption and transport in polymerâ€grafted ion exchangers: A multiscale modeling study. AICHE Journal, 2017, 63, 4564-4575.	3.6	10
36	Overview of the SAMPL5 hostâ€“guest challenge: Are we doing better?. Journal of Computer-Aided Molecular Design, 2017, 31, 1-19.	2.9	140

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37	Lessons learned from comparing molecular dynamics engines on the SAMPL5 dataset. Journal of Computer-Aided Molecular Design, 2017, 31, 147-161.	2.9	187
38	Blind prediction of cyclohexaneâ€“water distribution coefficients from the SAMPL5 challenge. Journal of Computer-Aided Molecular Design, 2016, 30, 927-944.	2.9	99
39	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, 3491-3505.	5.3	24
40	Rapid Computation of Thermodynamic Properties over Multidimensional Nonbonded Parameter Spaces Using Adaptive Multistate Reweighting. Journal of Chemical Theory and Computation, 2016, 12, 1806-1823.	5.3	13
41	Comparison of Methods To Reweight from Classical Molecular Simulations to QM/MM Potentials. Journal of Chemical Theory and Computation, 2016, 12, 1466-1480.	5.3	42
42	Identifying Differences and Similarities in Static and Dynamic Contact Angles between Nanoscale and Microscale Textured Surfaces Using Molecular Dynamics Simulations. Langmuir, 2015, 31, 7980-7990.	3.5	4
43	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, 2536-2549.	5.3	41
44	Guidelines for the analysis of free energy calculations. Journal of Computer-Aided Molecular Design, 2015, 29, 397-411.	2.9	375
45	Effects of Polymer Graft Properties on Protein Adsorption and Transport in Ion Exchange Chromatography: A Multiscale Modeling Study. Langmuir, 2015, 31, 4176-4187.	3.5	17
46	Converging free energies of binding in cucurbit[7]uril and octa-acid hostâ€“guest systems from SAMPL4 using expanded ensemble simulations. Journal of Computer-Aided Molecular Design, 2014, 28, 401-415.	2.9	39
47	Multiscale modeling of protein adsorption and transport in macroporous and polymerâ€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, 1128-1149.	5.3	33
49	Thermodynamics of Coupled Protein Adsorption and Stability Using Hybrid Monte Carlo Simulations. Langmuir, 2014, 30, 4952-4961.	3.5	7
50	Investigating the mutation resistance of nonnucleoside inhibitors of HIV-RT using multiple microsecond atomistic simulations. Proteins: Structure, Function and Bioinformatics, 2014, 82, 130-144.	2.6	5
51	Identifying ligand binding sites and poses using GPU-accelerated Hamiltonian replica exchange molecular dynamics. Journal of Computer-Aided Molecular Design, 2013, 27, 989-1007.	2.9	100
52	Simple Quantitative Tests to Validate Sampling from Thermodynamic Ensembles. Journal of Chemical Theory and Computation, 2013, 9, 909-926.	5.3	61
53	OpenMM 4: A Reusable, Extensible, Hardware Independent Library for High Performance Molecular Simulation. Journal of Chemical Theory and Computation, 2013, 9, 461-469.	5.3	583
54	GROMACS 4.5: a high-throughput and highly parallel open source molecular simulation toolkit. Bioinformatics, 2013, 29, 845-854.	4.1	6,072

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55	An Introduction to Best Practices in Free Energy Calculations. Methods in Molecular Biology, 2013, 924, 271-311.	0.9	84
56	Effects of Temperature Control Algorithms on Transport Properties and Kinetics in Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 2887-2899.	5.3	303
57	Glycoside Hydrolase Processivity Is Directly Related to Oligosaccharide Binding Free Energy. Journal of the American Chemical Society, 2013, 135, 18831-18839.	13.7	79
58	Using Multistate Reweighting to Rapidly and Efficiently Explore Molecular Simulation Parameters Space for Nonbonded Interactions. Journal of Chemical Theory and Computation, 2013, 9, 4700-4717.	5.3	14
59	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.	3.0	13
60	Product Binding Varies Dramatically between Processive and Nonprocessive Cellulase Enzymes. Journal of Biological Chemistry, 2012, 287, 24807-24813.	3.4	57
61	Configurational Preferences of Arylamide Î±-Helix Mimetics via Alchemical Free Energy Calculations of Relative Binding Affinities. Journal of Physical Chemistry B, 2012, 116, 10856-10869.	2.6	5
62	Optimal pairwise and non-pairwise alchemical pathways for free energy calculations of molecular transformation in solution phase. Journal of Chemical Physics, 2012, 136, 124120.	3.0	48
63	Distinct Aggregation Mechanisms of Monoclonal Antibody Under Thermal and Freeze-Thaw Stresses Revealed by Hydrogen Exchange. Pharmaceutical Research, 2012, 29, 236-250.	3.5	133
64	Best Practices in Free Energy Calculations for Drug Design. Methods in Molecular Biology, 2012, 819, 425-467.	0.9	36
65	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.	2.5	16
66	Identifying low variance pathways for free energy calculations of molecular transformations in solution phase. Journal of Chemical Physics, 2011, 135, 034114.	3.0	80
67	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, 4115-4134.	5.3	123
68	Alchemical free energy methods for drug discovery: progress and challenges. Current Opinion in Structural Biology, 2011, 21, 150-160.	5.7	468
69	Replica exchange and expanded ensemble simulations as Gibbs sampling: Simple improvements for enhanced mixing. Journal of Chemical Physics, 2011, 135, 194110.	3.0	137
70	Probing Carbohydrate Product Expulsion from a Processive Cellulase with Multiple Absolute Binding Free Energy Methods. Journal of Biological Chemistry, 2011, 286, 18161-18169.	3.4	69
71	Dynamical reweighting: Improved estimates of dynamical properties from simulations at multiple temperatures. Journal of Chemical Physics, 2011, 134, 244107.	3.0	55
72	Free-energy calculations in structure-based drug design. , 2010, , 61-86.		65

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73	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.	5.3	302
74	Statistically optimal analysis of samples from multiple equilibrium states. Journal of Chemical Physics, 2008, 129, 124105.	3.0	1,328
75	Chapter 4 Alchemical Free Energy Calculations: Ready for Prime Time?. Annual Reports in Computational Chemistry, 2007, 3, 41-59.	1.7	175
76	Accurate and Efficient Corrections for Missing Dispersion Interactions in Molecular Simulations. Journal of Physical Chemistry B, 2007, 111, 13052-13063.	2.6	181
77	Improved Methods for Side Chain and Loop Predictions via the Protein Local Optimization Program:â€‰Variable Dielectric Model for Implicitly Improving the Treatment of Polarization Effects. Journal of Chemical Theory and Computation, 2007, 3, 2108-2119.	5.3	104
78	Multiscale Optimization of a Truncated Newton Minimization Algorithm and Application to Proteins and Proteinâ˜Ligand Complexes. Journal of Chemical Theory and Computation, 2007, 3, 640-648.	5.3	29
79	Parallelized-over-parts computation of absolute binding free energy with docking and molecular dynamics. Journal of Chemical Physics, 2006, 125, 084901.	3.0	92
80	The Solvation Interface is a Determining Factor in Peptide Conformational Preferences. Journal of Molecular Biology, 2006, 356, 248-256.	4.2	44
81	Solvation free energies of amino acid side chain analogs for common molecular mechanics water models. Journal of Chemical Physics, 2005, 122, 134508.	3.0	357
82	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.	3.0	329
83	Direct calculation of the binding free energies of FKBP ligands. Journal of Chemical Physics, 2005, 123, 084108.	3.0	179
84	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.	3.0	611
85	Equilibrium Free Energies from Nonequilibrium Measurements Using Maximum-Likelihood Methods. Physical Review Letters, 2003, 91, 140601.	7.8	419
86	Deviations from the Boltzmann distribution in small microcanonical quantum systems: Two approximate one-particle energy distributions. Journal of Chemical Physics, 2002, 117, 5564-5575.	3.0	8
87	Native-like Mean Structure in the Unfolded Ensemble of Small Proteins. Journal of Molecular Biology, 2002, 323, 153-164.	4.2	168
88	Simulation of Folding of a Small Alpha-helical Protein in Atomistic Detail using Worldwide-distributed Computing. Journal of Molecular Biology, 2002, 323, 927-937.	4.2	266
89	Mathematical Analysis of Coupled Parallel Simulations. Physical Review Letters, 2001, 86, 4983-4987.	7.8	93