

Michael R Shirts

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.

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	GROMACS 4.5: a high-throughput and highly parallel open source molecular simulation toolkit. <i>Bioinformatics</i> , 2013 , 29, 845-54	7.2	4786
89	Statistically optimal analysis of samples from multiple equilibrium states. <i>Journal of Chemical Physics</i> , 2008 , 129, 124105	3.9	1012
88	Extremely precise free energy calculations of amino acid side chain analogs: Comparison of common molecular mechanics force fields for proteins. <i>Journal of Chemical Physics</i> , 2003 , 119, 5740-5761	3.9	544
87	OpenMM 4: A Reusable, Extensible, Hardware Independent Library for High Performance Molecular Simulation. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 461-469	6.4	440
86	Alchemical free energy methods for drug discovery: progress and challenges. <i>Current Opinion in Structural Biology</i> , 2011 , 21, 150-60	8.1	382
85	Equilibrium free energies from nonequilibrium measurements using maximum-likelihood methods. <i>Physical Review Letters</i> , 2003 , 91, 140601	7.4	360
84	Solvation free energies of amino acid side chain analogs for common molecular mechanics water models. <i>Journal of Chemical Physics</i> , 2005 , 122, 134508	3.9	329
83	Comparison of efficiency and bias of free energies computed by exponential averaging, the Bennett acceptance ratio, and thermodynamic integration. <i>Journal of Chemical Physics</i> , 2005 , 122, 144107	3.9	288
82	Guidelines for the analysis of free energy calculations. <i>Journal of Computer-Aided Molecular Design</i> , 2015 , 29, 397-411	4.2	281
81	Small molecule hydration free energies in explicit solvent: An extensive test of fixed-charge atomistic simulations. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 350-358	6.4	279
80	Simulation of folding of a small alpha-helical protein in atomistic detail using worldwide-distributed computing. <i>Journal of Molecular Biology</i> , 2002 , 323, 927-37	6.5	245
79	Effects of Temperature Control Algorithms on Transport Properties and Kinetics in Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 2887-99	6.4	213
78	Direct calculation of the binding free energies of FKBP ligands. <i>Journal of Chemical Physics</i> , 2005 , 123, 084108	3.9	165
77	Native-like mean structure in the unfolded ensemble of small proteins. <i>Journal of Molecular Biology</i> , 2002 , 323, 153-64	6.5	164
76	Chapter 4 Alchemical Free Energy Calculations: Ready for Prime Time?. <i>Annual Reports in Computational Chemistry</i> , 2007 , 3, 41-59	1.8	156
75	Accurate and efficient corrections for missing dispersion interactions in molecular simulations. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 13052-63	3.4	141
74	Distinct aggregation mechanisms of monoclonal antibody under thermal and freeze-thaw stresses revealed by hydrogen exchange. <i>Pharmaceutical Research</i> , 2012 , 29, 236-50	4.5	120

73	Replica exchange and expanded ensemble simulations as Gibbs sampling: simple improvements for enhanced mixing. <i>Journal of Chemical Physics</i> , 2011 , 135, 194110	3.9	118
72	Overview of the SAMPL5 host-guest challenge: Are we doing better?. <i>Journal of Computer-Aided Molecular Design</i> , 2017 , 31, 1-19	4.2	116
71	Approaches for calculating solvation free energies and enthalpies demonstrated with an update of the FreeSolv database. <i>Journal of Chemical & Engineering Data</i> , 2017 , 62, 1559-1569	2.8	114
70	A Benchmark Test Set for Alchemical Free Energy Transformations and Its Use to Quantify Error in Common Free Energy Methods. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 4115-34	6.4	99
69	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. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 2108-19	6.4	89
68	Mathematical analysis of coupled parallel simulations. <i>Physical Review Letters</i> , 2001 , 86, 4983-7	7.4	87
67	Identifying ligand binding sites and poses using GPU-accelerated Hamiltonian replica exchange molecular dynamics. <i>Journal of Computer-Aided Molecular Design</i> , 2013 , 27, 989-1007	4.2	86
66	Lessons learned from comparing molecular dynamics engines on the SAMPL5 dataset. <i>Journal of Computer-Aided Molecular Design</i> , 2017 , 31, 147-161	4.2	81
65	Parallelized-over-parts computation of absolute binding free energy with docking and molecular dynamics. <i>Journal of Chemical Physics</i> , 2006 , 125, 084901	3.9	81
64	Blind prediction of cyclohexane-water distribution coefficients from the SAMPL5 challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2016 , 30, 927-944	4.2	80
63	An introduction to best practices in free energy calculations. <i>Methods in Molecular Biology</i> , 2013 , 924, 271-311	1.4	72
62	Glycoside hydrolase processivity is directly related to oligosaccharide binding free energy. <i>Journal of the American Chemical Society</i> , 2013 , 135, 18831-9	16.4	71
61	Probing carbohydrate product expulsion from a processive cellulase with multiple absolute binding free energy methods. <i>Journal of Biological Chemistry</i> , 2011 , 286, 18161-9	5.4	64
60	Escaping Atom Types in Force Fields Using Direct Chemical Perception. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 6076-6092	6.4	62
59	Identifying low variance pathways for free energy calculations of molecular transformations in solution phase. <i>Journal of Chemical Physics</i> , 2011 , 135, 034114	3.9	61
58	Free-energy calculations in structure-based drug design		58
57	The SAMPL6 SAMPLing challenge: assessing the reliability and efficiency of binding free energy calculations. <i>Journal of Computer-Aided Molecular Design</i> , 2020 , 34, 601-633	4.2	55
56	Simple Quantitative Tests to Validate Sampling from Thermodynamic Ensembles. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 909-26	6.4	52

55	Dynamical reweighting: improved estimates of dynamical properties from simulations at multiple temperatures. <i>Journal of Chemical Physics</i> , 2011 , 134, 244107	3.9	50
54	Product binding varies dramatically between processive and nonprocessive cellulase enzymes. <i>Journal of Biological Chemistry</i> , 2012 , 287, 24807-13	5.4	49
53	The solvation interface is a determining factor in peptide conformational preferences. <i>Journal of Molecular Biology</i> , 2006 , 356, 248-56	6.5	40
52	Linear basis function approach to efficient alchemical free energy calculations. 2. Inserting and deleting particles with coulombic interactions. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 2536-49	6.4	39
51	Best Practices for Alchemical Free Energy Calculations [Article v1.0]. <i>Living Journal of Computational Molecular Science</i> , 2020 , 2,	10.1	38
50	Comparison of Methods To Reweight from Classical Molecular Simulations to QM/MM Potentials. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 1466-80	6.4	36
49	Optimal pairwise and non-pairwise alchemical pathways for free energy calculations of molecular transformation in solution phase. <i>Journal of Chemical Physics</i> , 2012 , 136, 124120	3.9	36
48	Capturing Entropic Contributions to Temperature-Mediated Polymorphic Transformations Through Molecular Modeling. <i>Crystal Growth and Design</i> , 2017 , 17, 1775-1787	3.5	34
47	Converging free energies of binding in cucurbit[7]uril and octa-acid host-guest systems from SAMPL4 using expanded ensemble simulations. <i>Journal of Computer-Aided Molecular Design</i> , 2014 , 28, 401-15	4.2	30
46	Linear Basis Function Approach to Efficient Alchemical Free Energy Calculations. 1. Removal of Uncharged Atomic Sites. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 1128-49	6.4	30
45	Best practices in free energy calculations for drug design. <i>Methods in Molecular Biology</i> , 2012 , 819, 425-674	6.7	28
44	Multiscale Optimization of a Truncated Newton Minimization Algorithm and Application to Proteins and Protein-Ligand Complexes. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 640-8	6.4	27
43	Toward Learned Chemical Perception of Force Field Typing Rules. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 402-423	6.4	23
42	Testing for physical validity in molecular simulations. <i>PLoS ONE</i> , 2018 , 13, e0202764	3.7	22
41	Effects of a More Accurate Polarizable Hamiltonian on Polymorph Free Energies Computed Efficiently by Reweighting Point-Charge Potentials. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 3491-505	6.4	19
40	Multiscale modeling of protein adsorption and transport in macroporous and polymer-grafted ion exchangers. <i>AIChE Journal</i> , 2014 , 60, 3888-3901	3.6	19
39	Configuration-Sampling-Based Surrogate Models for Rapid Parameterization of Non-Bonded Interactions. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 3144-3162	6.4	18
38	Exploring the Multi-minima Behavior of Small Molecule Crystal Polymorphs at Finite Temperature. <i>Crystal Growth and Design</i> , 2019 , 19, 5568-5580	3.5	16

37	Effects of polymer graft properties on protein adsorption and transport in ion exchange chromatography: a multiscale modeling study. <i>Langmuir</i> , 2015 , 31, 4176-87	4	15
36	Using Multistate Reweighting to Rapidly and Efficiently Explore Molecular Simulation Parameter Space for Nonbonded Interactions. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 4700-17	6.4	13
35	Modeling of arylamide helix mimetics in the p53 peptide binding site of hDM2 suggests parallel and anti-parallel conformations are both stable. <i>PLoS ONE</i> , 2012 , 7, e43253	3.7	13
34	Using reweighting and free energy surface interpolation to predict solid-solid phase diagrams. <i>Journal of Chemical Physics</i> , 2018 , 148, 144104	3.9	12
33	Development and Benchmarking of Open Force Field v1.0.0-the Parsley Small-Molecule Force Field. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 6262-6280	6.4	12
32	Open Force Field Consortium: Escaping atom types using direct chemical perception with SMIRNOFF v0.1		11
31	Effects of protein properties on adsorption and transport in polymer-grafted ion exchangers: A multiscale modeling study. <i>AICHE Journal</i> , 2017 , 63, 4564-4575	3.6	10
30	Rapid Computation of Thermodynamic Properties over Multidimensional Nonbonded Parameter Spaces Using Adaptive Multistate Reweighting. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 1806-23	6.4	10
29	Multistate reweighting and configuration mapping together accelerate the efficiency of thermodynamic calculations as a function of molecular geometry by orders of magnitude. <i>Journal of Chemical Physics</i> , 2013 , 138, 154108	3.9	9
28	Thermal Gradient Approach for the Quasi-harmonic Approximation and Its Application to Improved Treatment of Anisotropic Expansion. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 5904-5919	6.4	9
27	Adding Anisotropy to the Standard Quasi-Harmonic Approximation Still Fails in Several Ways to Capture Organic Crystal Thermodynamics. <i>Crystal Growth and Design</i> , 2019 , 19, 6911-6924	3.5	8
26	Understanding the Nanoscale Structure of Inverted Hexagonal Phase Lyotropic Liquid Crystal Polymer Membranes. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 289-309	3.4	8
25	Thermodynamics of coupled protein adsorption and stability using hybrid Monte Carlo simulations. <i>Langmuir</i> , 2014 , 30, 4952-61	4	7
24	Deviations from the Boltzmann distribution in small microcanonical quantum systems: Two approximate one-particle energy distributions. <i>Journal of Chemical Physics</i> , 2002 , 117, 5564-5575	3.9	7
23	Uncertainty quantification confirms unreliable extrapolation toward high pressures for united-atom Mie -6 force field. <i>Journal of Chemical Physics</i> , 2018 , 149, 114109	3.9	7
22	Chemically Selective Transport in a Cross-Linked H Phase Lyotropic Liquid Crystal Membrane. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 6314-6330	3.4	5
21	Investigating the mutation resistance of nonnucleoside inhibitors of HIV-RT using multiple microsecond atomistic simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014 , 82, 130-44	4.2	5
20	Configurational preferences of arylamide helix mimetics via alchemical free energy calculations of relative binding affinities. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 10856-69	3.4	5

19	Statistical Inference of Transport Mechanisms and Long Time Scale Behavior from Time Series of Solute Trajectories in Nanostructured Membranes. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 8110-8123 ^{3,4}	5
18	The SAMPL6 SAMPLing challenge: Assessing the reliability and efficiency of binding free energy calculations	4
17	Histogram-Free Reweighting with Grand Canonical Monte Carlo: Post-simulation Optimization of Non-bonded Potentials for Phase Equilibria. <i>Journal of Chemical & Engineering Data</i> , 2019 , 64, 3701-3717 ^{2,8}	3
16	Identifying Differences and Similarities in Static and Dynamic Contact Angles between Nanoscale and Microscale Textured Surfaces Using Molecular Dynamics Simulations. <i>Langmuir</i> , 2015 , 31, 7980-90	4 3
15	Statistically Optimal Continuous Free Energy Surfaces from Biased Simulations and Multistate Reweighting. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 4107-4125	6.4 3
14	Development and Benchmarking of Open Force Field v1.0.0, the Parsley Small Molecule Force Field	3
13	Statistical Mechanical Approximations to More Efficiently Determine Polymorph Free Energy Differences for Small Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 6503-6512 ^{6,4}	3
12	A nanostructured bifunctional acidBase catalyst resin formed by lyotropic liquid crystal monomers. <i>Canadian Journal of Chemistry</i> , 2020 , 98, 332-336	0.9 2
11	Adaptive Ensemble Biomolecular Applications at Scale. <i>SN Computer Science</i> , 2020 , 1, 1	2 2
10	Development and Benchmarking of Open Force Field v1.0.0, the Parsley Small Molecule Force Field	2
9	Development and Benchmarking of Open Force Field v1.0.0, the Parsley Small Molecule Force Field	2
8	Why We Need the Living Journal of Computational Molecular Science. <i>Living Journal of Computational Molecular Science</i> , 2019 , 1,	10.1 2
7	Lessons learned from comparing molecular dynamics engines on the SAMPL5 dataset	2
6	Capturing Subdiffusive Solute Dynamics and Predicting Selectivity in Nanoscale Pores with Time Series Modeling. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 5456-5473	6.4 2
5	Potential Foldamers Based on an Terphenyl Amino Acid. <i>Organic Letters</i> , 2021 , 23, 4855-4859	6.2 2
4	Expanded Ensemble Methods Can be Used to Accurately Predict Protein-Ligand Relative Binding Free Energies. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 6536-6547	6.4 1
3	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. <i>Journal of Chemical Physics</i> , 2019 , 150, 164112	3.9 0
2	Using a Coarse-Grained Modeling Framework to Identify Oligomeric Motifs with Tunable Secondary Structure. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 6018-6035	6.4 0

- 1 physical_validation: A Python package to assess the physical validity of molecular simulation results. *Journal of Open Source Software*, **2022**, 7, 3981 5.2