

# Andreas Krmer

## 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.

25  
papers

411  
citations

11  
h-index

20  
g-index

25  
ext. papers

639  
ext. citations

6.8  
avg, IF

4.44  
L-index

#	Paper	IF	Citations
25	Molecular Dynamics Simulations of Membrane Permeability. <i>Chemical Reviews</i> , <b>2019</b> , 119, 5954-5997	68.1	117
24	Permeability of membranes in the liquid ordered and liquid disordered phases. <i>Nature Communications</i> , <b>2019</b> , 10, 5616	17.4	37
23	Semi-Lagrangian off-lattice Boltzmann method for weakly compressible flows. <i>Physical Review E</i> , <b>2017</b> , 95, 023305	2.4	35
22	Coarse graining molecular dynamics with graph neural networks. <i>Journal of Chemical Physics</i> , <b>2020</b> , 153, 194101	3.9	34
21	TorchMD: A Deep Learning Framework for Molecular Simulations. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 2355-2363	6.4	23
20	Interactions of Water and Alkanes: Modifying Additive Force Fields to Account for Polarization Effects. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 3854-3867	6.4	19
19	Semi-Lagrangian lattice Boltzmann method for compressible flows. <i>Physical Review E</i> , <b>2020</b> , 101, 053306	2.4	19
18	Membrane permeability of small molecules from unbiased molecular dynamics simulations. <i>Journal of Chemical Physics</i> , <b>2020</b> , 153, 124107	3.9	15
17	Multistep lattice Boltzmann methods: Theory and applications. <i>International Journal for Numerical Methods in Fluids</i> , <b>2019</b> , 90, 156-169	1.9	15
16	Pseudoentropic derivation of the regularized lattice Boltzmann method. <i>Physical Review E</i> , <b>2019</b> , 100, 023302	2.4	13
15	Automated parameterization of intermolecular pair potentials using global optimization techniques. <i>Computer Physics Communications</i> , <b>2014</b> , 185, 3228-3239	4.2	12
14	Optimizing Molecular Models Through Force-Field Parameterization via the Efficient Combination of Modular Program Packages. <i>Molecular Modeling and Simulation</i> , <b>2016</b> , 53-77		10
13	Lattice Boltzmann simulations on irregular grids: Introduction of the NATrium library. <i>Computers and Mathematics With Applications</i> , <b>2020</b> , 79, 34-54	2.7	8
12	CHARMM36 Lipid Force Field with Explicit Treatment of Long-Range Dispersion: Parametrization and Validation for Phosphatidylethanolamine, Phosphatidylglycerol, and Ether Lipids. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 1581-1595	6.4	8
11	Optimized atomistic force fields for aqueous solutions of Magnesium and Calcium Chloride: Analysis, achievements and limitations. <i>European Physical Journal: Special Topics</i> , <b>2016</b> , 225, 1391-1409	2.3	7
10	Molecular dynamics simulations of ethanol permeation through single and double-lipid bilayers. <i>Journal of Chemical Physics</i> , <b>2020</b> , 153, 125101	3.9	7
9	Semi-automated Optimization of the CHARMM36 Lipid Force Field to Include Explicit Treatment of Long-Range Dispersion. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 1562-1580	6.4	6

8	Machine learning implicit solvation for molecular dynamics. <i>Journal of Chemical Physics</i> , <b>2021</b> , 155, 084101	6
7	Multi-phase Boltzmann weighting: accounting for local inhomogeneity in molecular simulations of water-octanol partition coefficients in the SAMPL6 challenge. <i>Journal of Computer-Aided Molecular Design</i> , <b>2020</b> , 34, 471-483	4.2 5
6	Transition point prediction in a multicomponent lattice Boltzmann model: Forcing scheme dependencies. <i>Physical Review E</i> , <b>2018</b> , 97, 023313	2.4 5
5	Permeation Rates of Oxygen through a Lipid Bilayer Using Replica Exchange Transition Interface Sampling. <i>Journal of Physical Chemistry B</i> , <b>2021</b> , 125, 193-201	3.4 5
4	Cubature rules for weakly and fully compressible off-lattice Boltzmann methods. <i>Journal of Computational Science</i> , <b>2021</b> , 51, 101355	3.4 4
3	High-order semi-Lagrangian kinetic scheme for compressible turbulence. <i>Physical Review E</i> , <b>2021</b> , 104, 025301	2.4 1
2	Lettuce: PyTorch-Based Lattice Boltzmann Framework. <i>Lecture Notes in Computer Science</i> , <b>2021</b> , 40-55	0.9 0
1	Molecular Dynamics Simulation of Membrane Free Energy Profiles Using Accurate Force Field for Ionic Liquids <b>2017</b> , 265-284	