Andreas Krmer

List of Publications by Year in Descending Order

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	Lettuce: PyTorch-Based Lattice Boltzmann Framework. *Lecture Notes in Computer Science*, **2021**, 40-55	0.9	0
24	Permeation Rates of Oxygen through a Lipid Bilayer Using Replica Exchange Transition Interface Sampling. *Journal of Physical Chemistry B*, **2021**, 125, 193-201	3.4	5
23	TorchMD: A Deep Learning Framework for Molecular Simulations. *Journal of Chemical Theory and Computation*, **2021**, 17, 2355-2363	6.4	23
22	Cubature rules for weakly and fully compressible off-lattice Boltzmann methods. *Journal of Computational Science*, **2021**, 51, 101355	3.4	4
21	CHARMM36 Lipid Force Field with Explicit Treatment of Long-Range Dispersion: Parametrization and Validation for Phosphatidylethanolamine, Phosphatidylglycerol, and Ether Lipids. *Journal of Chemical Theory and Computation*, **2021**, 17, 1581-1595	6.4	8
20	Semi-automated Optimization of the CHARMM36 Lipid Force Field to Include Explicit Treatment of Long-Range Dispersion. *Journal of Chemical Theory and Computation*, **2021**, 17, 1562-1580	6.4	6
19	High-order semi-Lagrangian kinetic scheme for compressible turbulence. *Physical Review E*, **2021**, 104, 025301	2.4	1
18	Machine learning implicit solvation for molecular dynamics. *Journal of Chemical Physics*, **2021**, 155, 084101	3.9	6
17	Semi-Lagrangian lattice Boltzmann method for compressible flows. *Physical Review E*, **2020**, 101, 053306	2.4	19
16	Multi-phase Boltzmann weighting: accounting for local inhomogeneity in molecular simulations of water-octanol partition coefficients in the SAMPL6 challenge. *Journal of Computer-Aided Molecular Design*, **2020**, 34, 471-483	4.2	5
15	Coarse graining molecular dynamics with graph neural networks. *Journal of Chemical Physics*, **2020**, 153, 194101	3.9	34
14	Molecular dynamics simulations of ethanol permeation through single and double-lipid bilayers. *Journal of Chemical Physics*, **2020**, 153, 125101	3.9	7
13	Membrane permeability of small molecules from unbiased molecular dynamics simulations. *Journal of Chemical Physics*, **2020**, 153, 124107	3.9	15
12	Lattice Boltzmann simulations on irregular grids: Introduction of the NATriuM library. *Computers and Mathematics With Applications*, **2020**, 79, 34-54	2.7	8
11	Interactions of Water and Alkanes: Modifying Additive Force Fields to Account for Polarization Effects. *Journal of Chemical Theory and Computation*, **2019**, 15, 3854-3867	6.4	19
10	Molecular Dynamics Simulations of Membrane Permeability. *Chemical Reviews*, **2019**, 119, 5954-5997	68.1	117
9	Pseudoentropic derivation of the regularized lattice Boltzmann method. *Physical Review E*, **2019**, 100, 023302	2.4	13

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8	Permeability of membranes in the liquid ordered and liquid disordered phases. *Nature Communications*, **2019**, 10, 5616	17.4	37
7	Multistep lattice Boltzmann methods: Theory and applications. *International Journal for Numerical Methods in Fluids*, **2019**, 90, 156-169	1.9	15
6	Transition point prediction in a multicomponent lattice Boltzmann model: Forcing scheme dependencies. *Physical Review E*, **2018**, 97, 023313	2.4	5
5	Semi-Lagrangian off-lattice Boltzmann method for weakly compressible flows. *Physical Review E*, **2017**, 95, 023305	2.4	35
4	Molecular Dynamics Simulation of Membrane Free Energy Profiles Using Accurate Force Field for Ionic Liquids **2017**, 265-284		
3	Optimized atomistic force fields for aqueous solutions of Magnesium and Calcium Chloride: Analysis, achievements and limitations. *European Physical Journal: Special Topics*, **2016**, 225, 1391-1409	2.3	7
2	Optimizing Molecular Models Through Force-Field Parameterization via the Efficient Combination of Modular Program Packages. *Molecular Modeling and Simulation*, **2016**, 53-77		10
1	Automated parameterization of intermolecular pair potentials using global optimization techniques. *Computer Physics Communications*, **2014**, 185, 3228-3239	4.2	12