Christoph Klein

List of Publications by Year
in descending order

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8 papers	2,456 citations	1306789 7 h-index	1588620 8 g-index
9 all docs	9 docs citations	9 times ranked	4006 citing authors

#	Article	IF	Citations
1	Formalizing atom-typing and the dissemination of force fields with foyer. Computational Materials Science, 2019, 167, 215-227.	1.4	29
2	Perfluoropolyethers: Development of an All-Atom Force Field for Molecular Simulations and Validation with New Experimental Vapor Pressures and Liquid Densities. Journal of Physical Chemistry B, 2017, 121, 6588-6600.	1.2	16
3	Lessons learned from comparing molecular dynamics engines on the SAMPL5 dataset. Journal of Computer-Aided Molecular Design, 2017, 31, 147-161.	1.3	187
4	A Hierarchical, Component Based Approach to Screening Properties of Soft Matter. Molecular Modeling and Simulation, 2016, , 79-92.	0.2	36
5	Tunable transition from hydration to monomer-supported lubrication in zwitterionic monolayers revealed by molecular dynamics simulation. Soft Matter, 2015, 11, 3340-3346.	1.2	22
6	MDTraj: A Modern Open Library for the Analysis of Molecular Dynamics Trajectories. Biophysical Journal, 2015, 109, 1528-1532.	0.2	1,576
7	Web- and Cloud-based Software Infrastructure for Materials Design. Procedia Computer Science, 2014, 29, 2034-2044.	1.2	7
8	OpenMM 4: A Reusable, Extensible, Hardware Independent Library for High Performance Molecular Simulation. Journal of Chemical Theory and Computation, 2013, 9, 461-469.	2.3	583