

Christoph Klein

List of Publications by Year in descending order

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8
papers

2,456
citations

1307594

7
h-index

1588992

8
g-index

9
all docs

9
docs citations

9
times ranked

4006
citing authors

#	ARTICLE	IF	CITATIONS
1	MDTraj: A Modern Open Library for the Analysis of Molecular Dynamics Trajectories. Biophysical Journal, 2015, 109, 1528-1532.	0.5	1,576
2	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
3	Lessons learned from comparing molecular dynamics engines on the SAMPL5 dataset. Journal of Computer-Aided Molecular Design, 2017, 31, 147-161.	2.9	187
4	A Hierarchical, Component Based Approach to Screening Properties of Soft Matter. Molecular Modeling and Simulation, 2016, , 79-92.	0.2	36
5	Formalizing atom-typing and the dissemination of force fields with foyer. Computational Materials Science, 2019, 167, 215-227.	3.0	29
6	Tunable transition from hydration to monomer-supported lubrication in zwitterionic monolayers revealed by molecular dynamics simulation. Soft Matter, 2015, 11, 3340-3346.	2.7	22
7	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.	2.6	16
8	Web- and Cloud-based Software Infrastructure for Materials Design. Procedia Computer Science, 2014, 29, 2034-2044.	2.0	7