Carsten Kutzner

List of Publications by Year
in descending order

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18	16,264	516710 16	839539 18
papers	citations	h-index	g-index

18	18	18	20359
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	GROMACS in the Cloud: A Global Supercomputer to Speed Up Alchemical Drug Design. Journal of Chemical Information and Modeling, 2022, 62, 1691-1711.	5.4	37
2	A CUDA fast multipole method with highly efficient M2L far field evaluation. International Journal of High Performance Computing Applications, 2021, 35, 97-117.	3.7	3
3	A GPU-Accelerated Fast Multipole Method for GROMACS: Performance and Accuracy. Journal of Chemical Theory and Computation, 2020, 16, 6938-6949.	5.3	68
4	GROMEX: A Scalable and Versatile Fast Multipole Method for Biomolecular Simulation. Lecture Notes in Computational Science and Engineering, 2020, , 517-543.	0.3	2
5	More bang for your buck: Improved use of GPU nodes for GROMACS 2018. Journal of Computational Chemistry, 2019, 40, 2418-2431.	3.3	286
6	GROmaïs: A GROMACS-Based Toolset to Analyze Density Maps Derived from Molecular Dynamics Simulations. Biophysical Journal, 2019, 116, 4-11.	0.5	73
7	Automated cryo-EM structure refinement using correlation-driven molecular dynamics. ELife, 2019, 8, .	6.0	83
8	Insights into the function of ion channels by computational electrophysiology simulations. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1741-1752.	2.6	60
9	Best bang for your buck: GPU nodes for <scp>GROMACS</scp> biomolecular simulations. Journal of Computational Chemistry, 2015, 36, 1990-2008.	3.3	195
10	Tackling Exascale Software Challenges in Molecular Dynamics Simulations with GROMACS. Lecture Notes in Computer Science, 2015, , 3-27.	1.3	581
11	Molecular Dynamics in Principal Component Space. Journal of Physical Chemistry B, 2012, 116, 8350-8354.	2.6	21
12	Computational Electrophysiology: The Molecular Dynamics of Ion Channel Permeation and Selectivity in Atomistic Detail. Biophysical Journal, 2011, 101, 809-817.	0.5	214
13	Keep It Flexible: Driving Macromolecular Rotary Motions in Atomistic Simulations with GROMACS. Journal of Chemical Theory and Computation, 2011, 7, 1381-1393.	5.3	42
14	Caught in the Act: Visualization of SNAREâ€Mediated Fusion Events in Molecular Detail. ChemBioChem, 2011, 12, 1049-1055.	2.6	134
15	GROMACS 4:â€‰ Algorithms for Highly Efficient, Load-Balanced, and Scalable Molecular Simulation. Journal of Chemical Theory and Computation, 2008, 4, 435-447.	5.3	13,875
16	Anatomy and Dynamics of a Supramolecular Membrane Protein Cluster. Science, 2007, 317, 1072-1076.	12.6	405
17	Speeding up parallel GROMACS on high-latency networks. Journal of Computational Chemistry, 2007, 28, 2075-2084.	3.3	107
18	effects of driving mechanisms in geodynamo models. Geophysical Research Letters, 2000, 27, 29-32.	4.0	78