Christoph Wehmeyer

List of Publications by Year
in descending order

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18	2,061	706676 14	889612 19
papers	citations	h-index	g-index

19	19	19	2711
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Machine Learning of Coarse-Grained Molecular Dynamics Force Fields. ACS Central Science, 2019, 5, 755-767.	5.3	306
2	Introduction to Markov state modeling with the PyEMMA software [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 1, .	2.2	45
3	Time-lagged autoencoders: Deep learning of slow collective variables for molecular kinetics. Journal of Chemical Physics, 2018, 148, 241703.	1.2	283
4	Markov state models from short non-equilibrium simulationsâ€”Analysis and correction of estimation bias. Journal of Chemical Physics, 2017, 146, .	1.2	51
5	Protein-peptide association kinetics beyond the seconds timescale from atomistic simulations. Nature Communications, 2017, 8, 1095.	5.8	137
6	Multiensemble Markov models of molecular thermodynamics and kinetics. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E3221-30.	3.3	173
7	MHC class II complexes sample intermediate states along the peptide exchange pathway. Nature Communications, 2016, 7, 13224.	5.8	40
8	The structure and IR signatures of the arginine-glutamate salt bridge. Insights from the classical MD simulations. Journal of Chemical Physics, 2015, 142, 215106.	1.2	18
9	PyEMMA 2: A Software Package for Estimation, Validation, and Analysis of Markov Models. Journal of Chemical Theory and Computation, 2015, 11, 5525-5542.	2.3	876
10	Efficient implementation and application of the artificial bee colony algorithm to low-dimensional optimization problems. Computer Physics Communications, 2014, 185, 1639-1646.	3.0	3
11	A Coupled Molecular Dynamics/Kinetic Monte Carlo Approach for Protonation Dynamics in Extended Systems. Journal of Chemical Theory and Computation, 2014, 10, 4221-4228.	2.3	19
12	Water-Free Proton Conduction in Hexakis(p-Phosphonatophenyl)benzene Nanochannels. Journal of Physical Chemistry C, 2013, 117, 12366-12372.	1.5	16
13	Foraging on the potential energy surface: A swarm intelligence-based optimizer for molecular geometry. Journal of Chemical Physics, 2012, 137, 194110.	1.2	8
14	Hydrogen bond networks: Structure and dynamics via firstâ€principles spectroscopy. Physica Status Solidi (B): Basic Research, 2012, 249, 368-375.	0.7	10
15	Artificial Bee Colony Optimization of Capping Potentials for Hybrid Quantum Mechanical/Molecular Mechanical Calculations. Journal of Chemical Theory and Computation, 2011, 7, 1307-1315.	2.3	24
16	Specific quantum mechanical/molecular mechanical capping-potentials for biomolecular functional groups. Journal of Chemical Physics, 2011, 135, 214107.	1.2	18
17	Isotopic Superlattices for Perfect Phonon Reflection. Journal of Electronic Materials, 2010, 39, 1769-1771.	1.0	7
18	Shock dynamics of two-lane driven lattice gases. Journal of Statistical Mechanics: Theory and Experiment, 2010, 2010, P06002.	0.9	24