Christoph Wehmeyer

List of Publications by Year
in descending order

18	2,061	623699 14	794568 19
papers	citations	h-index	g-index

19	19	19	2393
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	PyEMMA 2: A Software Package for Estimation, Validation, and Analysis of Markov Models. Journal of Chemical Theory and Computation, 2015, 11, 5525-5542.	5.3	876
2	Machine Learning of Coarse-Grained Molecular Dynamics Force Fields. ACS Central Science, 2019, 5, 755-767.	11.3	306
3	Time-lagged autoencoders: Deep learning of slow collective variables for molecular kinetics. Journal of Chemical Physics, 2018, 148, 241703.	3.0	283
4	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.	7.1	173
5	Protein-peptide association kinetics beyond the seconds timescale from atomistic simulations. Nature Communications, 2017, 8, 1095.	12.8	137
6	Markov state models from short non-equilibrium simulationsâ€”Analysis and correction of estimation bias. Journal of Chemical Physics, 2017, 146, .	3.0	51
7	Introduction to Markov state modeling with the PyEMMA software [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 1, .	6.4	45
8	MHC class II complexes sample intermediate states along the peptide exchange pathway. Nature Communications, 2016, 7, 13224.	12.8	40
9	Shock dynamics of two-lane driven lattice gases. Journal of Statistical Mechanics: Theory and Experiment, 2010, 2010, P06002.	2.3	24
10	Artificial Bee Colony Optimization of Capping Potentials for Hybrid Quantum Mechanical/Molecular Mechanical Calculations. Journal of Chemical Theory and Computation, 2011, 7, 1307-1315.	5.3	24
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.	5.3	19
12	Specific quantum mechanical/molecular mechanical capping-potentials for biomolecular functional groups. Journal of Chemical Physics, 2011, 135, 214107.	3.0	18
13	The structure and IR signatures of the arginine-glutamate salt bridge. Insights from the classical MD simulations. Journal of Chemical Physics, 2015, 142, 215106.	3.0	18
14	Water-Free Proton Conduction in Hexakis(p-Phosphonatophenyl)benzene Nanochannels. Journal of Physical Chemistry C, 2013, 117, 12366-12372.	3.1	16
15	Hydrogen bond networks: Structure and dynamics via firstâ€principles spectroscopy. Physica Status Solidi (B): Basic Research, 2012, 249, 368-375.	1.5	10
16	Foraging on the potential energy surface: A swarm intelligence-based optimizer for molecular geometry. Journal of Chemical Physics, 2012, 137, 194110.	3.0	8
17	Isotopic Superlattices for Perfect Phonon Reflection. Journal of Electronic Materials, 2010, 39, 1769-1771.	2.2	7
18	Efficient implementation and application of the artificial bee colony algorithm to low-dimensional optimization problems. Computer Physics Communications, 2014, 185, 1639-1646.	7.5	3