

Michael Gastegger

List of Publications by Year in descending order

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Version: 2024-02-01

19
papers

2,739
citations

430874

18
h-index

794594

19
g-index

19
all docs

19
docs citations

19
times ranked

2168
citing authors

#	ARTICLE	IF	CITATIONS
1	Machine Learning Force Fields. <i>Chemical Reviews</i> , 2021, 121, 10142-10186.	47.7	528
2	Machine learning molecular dynamics for the simulation of infrared spectra. <i>Chemical Science</i> , 2017, 8, 6924-6935.	7.4	349
3	Combining Machine Learning and Computational Chemistry for Predictive Insights Into Chemical Systems. <i>Chemical Reviews</i> , 2021, 121, 9816-9872.	47.7	287
4	Unifying machine learning and quantum chemistry with a deep neural network for molecular wavefunctions. <i>Nature Communications</i> , 2019, 10, 5024.	12.8	282
5	SchNetPack: A Deep Learning Toolbox For Atomistic Systems. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 448-455.	5.3	240
6	wACSFâ€”Weighted atom-centered symmetry functions as descriptors in machine learning potentials. <i>Journal of Chemical Physics</i> , 2018, 148, 241709.	3.0	198
7	Machine learning enables long time scale molecular photodynamics simulations. <i>Chemical Science</i> , 2019, 10, 8100-8107.	7.4	140
8	Combining SchNet and SHARC: The SchNarc Machine Learning Approach for Excited-State Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3828-3834.	4.6	114
9	SpookyNet: Learning force fields with electronic degrees of freedom and nonlocal effects. <i>Nature Communications</i> , 2021, 12, 7273.	12.8	108
10	Perspective on integrating machine learning into computational chemistry and materials science. <i>Journal of Chemical Physics</i> , 2021, 154, 230903.	3.0	107
11	High-Dimensional Neural Network Potentials for Organic Reactions and an Improved Training Algorithm. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2187-2198.	5.3	105
12	Inverse design of 3d molecular structures with conditional generative neural networks. <i>Nature Communications</i> , 2022, 13, 973.	12.8	70
13	Comparing the accuracy of high-dimensional neural network potentials and the systematic molecular fragmentation method: A benchmark study for all-trans alkanes. <i>Journal of Chemical Physics</i> , 2016, 144, 194110.	3.0	48
14	Machine learning of solvent effects on molecular spectra and reactions. <i>Chemical Science</i> , 2021, 12, 11473-11483.	7.4	47
15	A deep neural network for molecular wave functions in quasi-atomic minimal basis representation. <i>Journal of Chemical Physics</i> , 2020, 153, 044123.	3.0	34
16	Loganin and secologanin derived tryptamineâ€”iridoid alkaloids from <i>Palicourea crocea</i> and <i>Palicourea padifolia</i> (Rubiaceae). <i>Phytochemistry</i> , 2015, 116, 162-169.	2.9	28
17	Molecular force fields with gradient-domain machine learning (GDML): Comparison and synergies with classical force fields. <i>Journal of Chemical Physics</i> , 2020, 153, 124109.	3.0	25
18	Deep learning study of tyrosine reveals that roaming can lead to photodamage. <i>Nature Chemistry</i> , 2022, 14, 914-919.	13.6	21

#	ARTICLE	IF	CITATIONS
19	Exploring density functional subspaces with genetic algorithms. Monatshefte für Chemie, 2019, 150, 173-182.	1.8	8