Michael Gastegger

List of Publications by Year
in descending order

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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	Inverse design of 3d molecular structures with conditional generative neural networks. Nature Communications, 2022, 13, 973.	12.8	70
2	Deep learning study of tyrosine reveals that roaming can lead to photodamage. Nature Chemistry, 2022, 14, 914-919.	13.6	21
3	Machine learning of solvent effects on molecular spectra and reactions. Chemical Science, 2021, 12, 11473-11483.	7.4	47
4	Machine Learning Force Fields. Chemical Reviews, 2021, 121, 10142-10186.	47.7	528
5	Perspective on integrating machine learning into computational chemistry and materials science. Journal of Chemical Physics, 2021, 154, 230903.	3.0	107
6	Combining Machine Learning and Computational Chemistry for Predictive Insights Into Chemical Systems. Chemical Reviews, 2021, 121, 9816-9872.	47.7	287
7	SpookyNet: Learning force fields with electronic degrees of freedom and nonlocal effects. Nature Communications, 2021, 12, 7273.	12.8	108
8	Molecular force fields with gradient-domain machine learning (GDML): Comparison and synergies with classical force fields. Journal of Chemical Physics, 2020, 153, 124109.	3.0	25
9	A deep neural network for molecular wave functions in quasi-atomic minimal basis representation. Journal of Chemical Physics, 2020, 153, 044123.	3.0	34
10	Combining SchNet and SHARC: The SchNarc Machine Learning Approach for Excited-State Dynamics. Journal of Physical Chemistry Letters, 2020, 11, 3828-3834.	4.6	114
11	Machine learning enables long time scale molecular photodynamics simulations. Chemical Science, 2019, 10, 8100-8107.	7.4	140
12	Unifying machine learning and quantum chemistry with a deep neural network for molecular wavefunctions. Nature Communications, 2019, 10, 5024.	12.8	282
13	Exploring density functional subspaces with genetic algorithms. Monatshefte FÃ¼r Chemie, 2019, 150, 173-182.	1.8	8
14	SchNetPack: A Deep Learning Toolbox For Atomistic Systems. Journal of Chemical Theory and Computation, 2019, 15, 448-455.	5.3	240
15	wACSFâ€"Weighted atom-centered symmetry functions as descriptors in machine learning potentials. Journal of Chemical Physics, 2018, 148, 241709.	3.0	198
16	Machine learning molecular dynamics for the simulation of infrared spectra. Chemical Science, 2017, 8, 6924-6935.	7.4	349
17	Comparing the accuracy of high-dimensional neural network potentials and the systematic molecular fragmentation method: A benchmark study for all-trans alkanes. Journal of Chemical Physics, 2016, 144, 194110.	3.0	48
18	Loganin and secologanin derived tryptamineâ€“iridoid alkaloids from Palicourea crocea and Palicourea padifolia (Rubiaceae). Phytochemistry, 2015, 116, 162-169.	2.9	28

#	Article	IF	Citations
19	High-Dimensional Neural Network Potentials for Organic Reactions and an Improved Training Algorithm. Journal of Chemical Theory and Computation, 2015, 11, 2187-2198.	5.3	105