

List of Publications by Year in descending order

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12
papers

1,078
citations

840728

11
h-index

1199563

12
g-index

12
all docs

12
docs citations

12
times ranked

1256
citing authors

#	ARTICLE	IF	CITATIONS
1	Efficient implementation of atom-density representations. Journal of Chemical Physics, 2021, 154, 114109.	3.0	32
2	Physics-Inspired Structural Representations for Molecules and Materials. Chemical Reviews, 2021, 121, 9759-9815.	47.7	247
3	Optimal radial basis for density-based atomic representations. Journal of Chemical Physics, 2021, 155, 104106.	3.0	17
4	Atom-density representations for machine learning. Journal of Chemical Physics, 2019, 150, 154110.	3.0	120
5	Data Science Based Mg Corrosion Engineering. Frontiers in Materials, 2019, 6, .	2.4	34
6	Machine Learning at the Atomic Scale. Chimia, 2019, 73, 972.	0.6	4
7	Fast and Accurate Uncertainty Estimation in Chemical Machine Learning. Journal of Chemical Theory and Computation, 2019, 15, 906-915.	5.3	102
8	Machine learning for the structureâ€“energyâ€“property landscapes of molecular crystals. Chemical Science, 2018, 9, 1289-1300.	7.4	153
9	Feature optimization for atomistic machine learning yields a data-driven construction of the periodic table of the elements. Physical Chemistry Chemical Physics, 2018, 20, 29661-29668.	2.8	88
10	Chemical shifts in molecular solids by machine learning. Nature Communications, 2018, 9, 4501.	12.8	170
11	Mapping and classifying molecules from a high-throughput structural database. Journal of Cheminformatics, 2017, 9, 6.	6.1	28
12	The GBS code for tokamak scrape-off layer simulations. Journal of Computational Physics, 2016, 315, 388-408.	3.8	83