Jonathan Schmidt

List of Publications by Year
in descending order

14 papers	1,879 citations	933447 10 h-index	1058476 14 g-index
14 all docs	14 docs citations	14 times ranked	2726 citing authors

#	Article	IF	Citations
1	Recent advances and applications of machine learning in solid-state materials science. Npj Computational Materials, 2019, 5, .	8.7	1,289
2	Predicting the Thermodynamic Stability of Solids Combining Density Functional Theory and Machine Learning. Chemistry of Materials, 2017, 29, 5090-5103.	6.7	217
3	Exchange-correlation functionals for band gaps of solids: benchmark, reparametrization and machine learning. Npj Computational Materials, 2020, 6, .	8.7	156
4	Machine Learning the Physical Nonlocal Exchangeâ€“Correlation Functional of Density-Functional Theory. Journal of Physical Chemistry Letters, 2019, 10, 6425-6431.	4.6	62
5	Crystal graph attention networks for the prediction of stable materials. Science Advances, 2021, 7, eabi7948.	10.3	37
6	Predicting the stability of ternary intermetallics with density functional theory and machine learning. Journal of Chemical Physics, 2018, 148, 241728.	3.0	30
7	Reduced density matrix functional theory for superconductors. Physical Review B, 2019, 99, .	3.2	18
8	A high-throughput study of oxynitride, oxyfluoride and nitrofluoride perovskites. Journal of Materials Chemistry A, 2021, 9, 8501-8513.	10.3	18
9	Machine learning universal bosonic functionals. Physical Review Research, 2021, 3, .	3.6	11
10	Superconductivity in antiperovskites. Npj Computational Materials, 2022, 8, .	8.7	11
11	Machine learning the derivative discontinuity of density-functional theory. Machine Learning: Science and Technology, 2022, 3, 015011.	5.0	10
12	A dataset of 175k stable and metastable materials calculated with the PBEsol and SCAN functionals. Scientific Data, 2022, 9, 64.	5.3	8
13	Machine-learning correction to density-functional crystal structure optimization. MRS Bulletin, 2022, 47, 765-771.	3.5	7
14	Representability problem of density functional theory for superconductors. Physical Review B, 2019, 99, .	3.2	5