Daniel W Davies

List of Publications by Year
in descending order

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15	2,814	840776 11	996975 15
papers	citations	h-index	g-index

15	15	15	4274
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Breaking the Aristotype: Featurization of Polyhedral Distortions in Perovskite Crystals. Chemistry of Materials, 2022, 34, 562-573.	6.7	8
2	Investigation of factors affecting the stability of compounds formed by isovalent substitution in layered oxychalcogenides, leading to identification of Ba₃Sc₂O₅Cu₂Se₂, Ba₃Y₂O₅Cu₂S₂, Ba₃Sc₂O₅Ag₂Se₂ and Ba₃In₂O₅Ag₂Se₂. Journal of Materials Ch	5.5	1
3	Surfaxe: Systematic surface calculations. Journal of Open Source Software, 2021, 6, 3171.	4.6	13
4	Descriptors for Electron and Hole Charge Carriers in Metal Oxides. Journal of Physical Chemistry Letters, 2020, 11, 438-444.	4.6	22
5	Bandgap lowering in mixed alloys of Cs₂Ag(Sb_xBi_{1â^'x})Br₆ double perovskite thin films. Journal of Materials Chemistry A, 2020, 8, 21780-21788.	10.3	66
6	Modeling the dielectric constants of crystals using machine learning. Journal of Chemical Physics, 2020, 153, 024503.	3.0	29
7	Low-cost descriptors of electrostatic and electronic contributions to anion redox activity in batteries. IOP SciNotes, 2020, 1, 024805.	0.8	5
8	Data-Driven Discovery of Photoactive Quaternary Oxides Using First-Principles Machine Learning. Chemistry of Materials, 2019, 31, 7221-7230.	6.7	45
9	Identification of Lone-Pair Surface States on Indium Oxide. Journal of Physical Chemistry C, 2019, 123, 1700-1709.	3.1	20
10	SMACT: Semiconducting Materials by Analogy and Chemical Theory. Journal of Open Source Software, 2019, 4, 1361.	4.6	21
11	Materials discovery by chemical analogy: role of oxidation states in structure prediction. Faraday Discussions, 2018, 211, 553-568.	3.2	22
12	Computer-aided design of metal chalcohalide semiconductors: from chemical composition to crystal structure. Chemical Science, 2018, 9, 1022-1030.	7.4	54
13	Applications of crystal structure prediction â€“ inorganic and network structures: general discussion. Faraday Discussions, 2018, 211, 613-642.	3.2	6
14	Machine learning for molecular and materials science. Nature, 2018, 559, 547-555.	27.8	2,387
15	Computational Screening of All Stoichiometric Inorganic Materials. CheM, 2016, 1, 617-627.	11.7	115