

Daniel W Davies

List of Publications by Year in descending order

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Version: 2024-02-01

15
papers

2,814
citations

840776

11
h-index

996975

15
g-index

15
all docs

15
docs citations

15
times ranked

4274
citing authors

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