Cormac Toher

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	High-entropy ceramics. Nature Reviews Materials, 2020, 5, 295-309.	48.7	902
2	Charting the complete elastic properties of inorganic crystalline compounds. Scientific Data, 2015, 2, 150009.	5.3	642
3	High-entropy high-hardness metal carbides discovered by entropy descriptors. Nature Communications, 2018, 9, 4980.	12.8	604
4	Universal fragment descriptors for predicting properties of inorganic crystals. Nature Communications, 2017, 8, 15679.	12.8	435
5	Phase stability and mechanical properties of novel high entropy transition metal carbides. Acta Materialia, 2019, 166, 271-280.	7.9	422
6	The AFLOW standard for high-throughput materials science calculations. Computational Materials Science, 2015, 108, 233-238.	3.0	244
7	High-throughput computational screening of thermal conductivity, Debye temperature, and Grüneisen parameter using a quasiharmonic Debye model. Physical Review B, 2014, 90, .	3.2	230
8	Machine learning for alloys. Nature Reviews Materials, 2021, 6, 730-755.	48.7	202
9	On-the-fly closed-loop materials discovery via Bayesian active learning. Nature Communications, 2020, 11, 5966.	12.8	167
10	A RESTful API for exchanging materials data in the AFLOWLIB.org consortium. Computational Materials Science, 2014, 93, 178-192.	3.0	148
11	The AFLOW Library of Crystallographic Prototypes: Part 1. Computational Materials Science, 2017, 136, S1-S828.	3.0	147
12	The search for high entropy alloys: A high-throughput ab-initio approach. Acta Materialia, 2018, 159, 364-383.	7.9	142
13	Discovery of high-entropy ceramics via machine learning. Npj Computational Materials, 2020, 6, .	8.7	133
14	Spectral descriptors for bulk metallic glasses based on the thermodynamics of competing crystalline phases. Nature Communications, 2016, 7, 12315.	12.8	104
15	Charge compensation and electrostatic transferability in three entropy-stabilized oxides: Results from density functional theory calculations. Journal of Applied Physics, 2016, 120, .	2.5	100
16	Predicting superhard materials via a machine learning informed evolutionary structure search. Npj Computational Materials, 2019, 5, .	8.7	74
17	AFLOW-ML: A RESTful API for machine-learning predictions of materials properties. Computational Materials Science, 2018, 152, 134-145.	3.0	72
18	The AFLOW Library of Crystallographic Prototypes: Part 2. Computational Materials Science, 2019, 161, \$1-\$1011.	3.0	70

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19	AFLOWÏ€: A minimalist approach to high-throughput ab initio calculations including the generation of tight-binding hamiltonians. Computational Materials Science, 2017, 136, 76-84.	3.0	70
20	AFLOW-CHULL: Cloud-Oriented Platform for Autonomous Phase Stability Analysis. Journal of Chemical Information and Modeling, 2018, 58, 2477-2490.	5.4	69
21	An efficient and accurate framework for calculating lattice thermal conductivity of solids: AFLOW—AAPL Automatic Anharmonic Phonon Library. Npj Computational Materials, 2017, 3, .	8.7	65
22	Unavoidable disorder and entropy in multi-component systems. Npj Computational Materials, 2019, 5, .	8.7	61
23	AFLUX: The LUX materials search API for the AFLOW data repositories. Computational Materials Science, 2017, 137, 362-370.	3.0	56
24	Combining the AFLOW GIBBS and elastic libraries to efficiently and robustly screen thermomechanical properties of solids. Physical Review Materials, 2017, 1, .	2.4	47
25	<i>AFLOW-SYM</i> : platform for the complete, automatic and self-consistent symmetry analysis of crystals. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, 184-203.	0.1	44
26	Coordination corrected ab initio formation enthalpies. Npj Computational Materials, 2019, 5, .	8.7	38
27	Entropy Landscaping of Highâ€Entropy Carbides. Advanced Materials, 2021, 33, e2102904.	21.0	38
28	XtalOptÂVersion r12: An open-source evolutionary algorithm for crystal structure prediction. Computer Physics Communications, 2019, 237, 274-275.	7.5	37
29	Data-driven design of inorganic materials with the Automatic Flow Framework for Materials Discovery. MRS Bulletin, 2018, 43, 670-675.	3.5	35
30	AFLOW-XtalFinder: a reliable choice to identify crystalline prototypes. Npj Computational Materials, 2021, 7, .	8.7	28
31	Carbon stoichiometry and mechanical properties of high entropy carbides. Acta Materialia, 2021, 215, 117051.	7.9	28
32	Settling the matter of the role of vibrations in the stability of high-entropy carbides. Nature Communications, 2021, 12, 5747.	12.8	28
33	High-entropy ceramics: Propelling applications through disorder. MRS Bulletin, 2022, 47, 194-202.	3.5	26
34	Metallic glasses for biodegradable implants. Acta Materialia, 2019, 176, 297-305.	7.9	25
35	The AFLOW Library of Crystallographic Prototypes: Part 3. Computational Materials Science, 2021, 199, 110450.	3.0	16
36	Molybdenum-titanium phase diagram evaluated from <i>ab initio</i> calculations. Physical Review Materials, 2017, 1, .	2.4	11

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37	Automated coordination corrected enthalpies with AFLOW-CCE. Physical Review Materials, 2021, 5, .	2.4	9
38	Spinodal Superlattices of Topological Insulators. Chemistry of Materials, 2018, 30, 2331-2340.	6.7	8
39	AFLOW-QHA3P: Robust and automated method to compute thermodynamic properties of solids. Physical Review Materials, 2019, 3, .	2.4	8
40	Physics in the Machine: Integrating Physical Knowledge in Autonomous Phase-Mapping. Frontiers in Physics, 2022, 10, .	2.1	6
41	The Microscopic Diamond Anvil Cell: Stabilization of Superhard, Superconducting Carbon Allotropes at Ambient Pressure. Angewandte Chemie - International Edition, 2022, 61, .	13.8	5
42	The Microscopic Diamond Anvil Cell: Stabilization of Superhard, Superconducting Carbon Allotropes at Ambient Pressure. Angewandte Chemie, 2022, 134, .	2.0	3