

# Cormac Toher

## List of Publications by Year in descending order

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42  
papers

5,601  
citations

172457

29  
h-index

265206

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g-index

43  
all docs

43  
docs citations

43  
times ranked

5235  
citing authors

#	ARTICLE	IF	CITATIONS
1	Physics in the Machine: Integrating Physical Knowledge in Autonomous Phase-Mapping. <i>Frontiers in Physics</i> , 2022, 10, .	2.1	6
2	High-entropy ceramics: Propelling applications through disorder. <i>MRS Bulletin</i> , 2022, 47, 194-202.	3.5	26
3	The Microscopic Diamond Anvil Cell: Stabilization of Superhard, Superconducting Carbon Allotropes at Ambient Pressure. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	13.8	5
4	The Microscopic Diamond Anvil Cell: Stabilization of Superhard, Superconducting Carbon Allotropes at Ambient Pressure. <i>Angewandte Chemie</i> , 2022, 134, .	2.0	3
5	AFLOW-XtalFinder: a reliable choice to identify crystalline prototypes. <i>Npj Computational Materials</i> , 2021, 7, .	8.7	28
6	Automated coordination corrected enthalpies with AFLOW-CCE. <i>Physical Review Materials</i> , 2021, 5, .	2.4	9
7	Machine learning for alloys. <i>Nature Reviews Materials</i> , 2021, 6, 730-755.	48.7	202
8	Carbon stoichiometry and mechanical properties of high entropy carbides. <i>Acta Materialia</i> , 2021, 215, 117051.	7.9	28
9	Entropy Landscaping of High-Entropy Carbides. <i>Advanced Materials</i> , 2021, 33, e2102904.	21.0	38
10	Settling the matter of the role of vibrations in the stability of high-entropy carbides. <i>Nature Communications</i> , 2021, 12, 5747.	12.8	28
11	The AFLOW Library of Crystallographic Prototypes: Part 3. <i>Computational Materials Science</i> , 2021, 199, 110450.	3.0	16
12	On-the-fly closed-loop materials discovery via Bayesian active learning. <i>Nature Communications</i> , 2020, 11, 5966.	12.8	167
13	High-entropy ceramics. <i>Nature Reviews Materials</i> , 2020, 5, 295-309.	48.7	902
14	Discovery of high-entropy ceramics via machine learning. <i>Npj Computational Materials</i> , 2020, 6, .	8.7	133
15	Unavoidable disorder and entropy in multi-component systems. <i>Npj Computational Materials</i> , 2019, 5, .	8.7	61
16	Metallic glasses for biodegradable implants. <i>Acta Materialia</i> , 2019, 176, 297-305.	7.9	25
17	Predicting superhard materials via a machine learning informed evolutionary structure search. <i>Npj Computational Materials</i> , 2019, 5, .	8.7	74
18	The AFLOW Library of Crystallographic Prototypes: Part 2. <i>Computational Materials Science</i> , 2019, 161, S1-S1011.	3.0	70

#	ARTICLE	IF	CITATIONS
19	Coordination corrected ab initio formation enthalpies. <i>Npj Computational Materials</i> , 2019, 5, .	8.7	38
20	Phase stability and mechanical properties of novel high entropy transition metal carbides. <i>Acta Materialia</i> , 2019, 166, 271-280.	7.9	422
21	XtalOpt Version r1.2: An open-source evolutionary algorithm for crystal structure prediction. <i>Computer Physics Communications</i> , 2019, 237, 274-275.	7.5	37
22	AFLOW-QHA3P: Robust and automated method to compute thermodynamic properties of solids. <i>Physical Review Materials</i> , 2019, 3, .	2.4	8
23	<i>AFLOW-SYM</i> : platform for the complete, automatic and self-consistent symmetry analysis of crystals. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2018, 74, 184-203.	0.1	44
24	Spinodal Superlattices of Topological Insulators. <i>Chemistry of Materials</i> , 2018, 30, 2331-2340.	6.7	8
25	High-entropy high-hardness metal carbides discovered by entropy descriptors. <i>Nature Communications</i> , 2018, 9, 4980.	12.8	604
26	AFLOW-CHULL: Cloud-Oriented Platform for Autonomous Phase Stability Analysis. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 2477-2490.	5.4	69
27	Data-driven design of inorganic materials with the Automatic Flow Framework for Materials Discovery. <i>MRS Bulletin</i> , 2018, 43, 670-675.	3.5	35
28	AFLOW-ML: A RESTful API for machine-learning predictions of materials properties. <i>Computational Materials Science</i> , 2018, 152, 134-145.	3.0	72
29	The search for high entropy alloys: A high-throughput ab-initio approach. <i>Acta Materialia</i> , 2018, 159, 364-383.	7.9	142
30	The AFLOW Library of Crystallographic Prototypes: Part 1. <i>Computational Materials Science</i> , 2017, 136, S1-S828.	3.0	147
31	An efficient and accurate framework for calculating lattice thermal conductivity of solids: AFLOW's APL Automatic Anharmonic Phonon Library. <i>Npj Computational Materials</i> , 2017, 3, .	8.7	65
32	AFLUX: The LUX materials search API for the AFLOW data repositories. <i>Computational Materials Science</i> , 2017, 137, 362-370.	3.0	56
33	Universal fragment descriptors for predicting properties of inorganic crystals. <i>Nature Communications</i> , 2017, 8, 15679.	12.8	435
34	AFLOW's: A minimalist approach to high-throughput ab initio calculations including the generation of tight-binding hamiltonians. <i>Computational Materials Science</i> , 2017, 136, 76-84.	3.0	70
35	Combining the AFLOW GIBBS and elastic libraries to efficiently and robustly screen thermomechanical properties of solids. <i>Physical Review Materials</i> , 2017, 1, .	2.4	47
36	Molybdenum-titanium phase diagram evaluated from ab initio calculations. <i>Physical Review Materials</i> , 2017, 1, .	2.4	11

#	ARTICLE	IF	CITATIONS
37	Charge compensation and electrostatic transferability in three entropy-stabilized oxides: Results from density functional theory calculations. <i>Journal of Applied Physics</i> , 2016, 120, .	2.5	100
38	Spectral descriptors for bulk metallic glasses based on the thermodynamics of competing crystalline phases. <i>Nature Communications</i> , 2016, 7, 12315.	12.8	104
39	The AFLOW standard for high-throughput materials science calculations. <i>Computational Materials Science</i> , 2015, 108, 233-238.	3.0	244
40	Charting the complete elastic properties of inorganic crystalline compounds. <i>Scientific Data</i> , 2015, 2, 150009.	5.3	642
41	High-throughput computational screening of thermal conductivity, Debye temperature, and Grüneisen parameter using a quasiharmonic Debye model. <i>Physical Review B</i> , 2014, 90, .	3.2	230
42	A RESTful API for exchanging materials data in the AFLOWLIB.org consortium. <i>Computational Materials Science</i> , 2014, 93, 178-192.	3.0	148