

# Stefano Curtarolo

## List of Publications by Year in descending order

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169  
papers

20,478  
citations

19657

61  
h-index

10158

140  
g-index

181  
all docs

181  
docs citations

181  
times ranked

18032  
citing authors

#	ARTICLE	IF	CITATIONS
1	Entropy-stabilized oxides. Nature Communications, 2015, 6, 8485.	12.8	1,624
2	The high-throughput highway to computational materials design. Nature Materials, 2013, 12, 191-201.	27.5	1,475
3	High-throughput electronic band structure calculations: Challenges and tools. Computational Materials Science, 2010, 49, 299-312.	3.0	1,140
4	High-entropy ceramics. Nature Reviews Materials, 2020, 5, 295-309.	48.7	902
5	AFLOW: An automatic framework for high-throughput materials discovery. Computational Materials Science, 2012, 58, 218-226.	3.0	898
6	AFLOWLIB.ORG: A distributed materials properties repository from high-throughput ab initio calculations. Computational Materials Science, 2012, 58, 227-235.	3.0	811
7	All The Catalytic Active Sites of MoS <sub>2</sub> for Hydrogen Evolution. Journal of the American Chemical Society, 2016, 138, 16632-16638.	13.7	664
8	Charting the complete elastic properties of inorganic crystalline compounds. Scientific Data, 2015, 2, 150009.	5.3	642
9	High-entropy high-hardness metal carbides discovered by entropy descriptors. Nature Communications, 2018, 9, 4980.	12.8	604
10	Convergence of multi-valley bands as the electronic origin of high thermoelectric performance in CoSb <sub>3</sub> skutterudites. Nature Materials, 2015, 14, 1223-1228.	27.5	587
11	Universal fragment descriptors for predicting properties of inorganic crystals. Nature Communications, 2017, 8, 15679.	12.8	435
12	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	38.1	427
13	Phase stability and mechanical properties of novel high entropy transition metal carbides. Acta Materialia, 2019, 166, 271-280.	7.9	422
14	Predicting Crystal Structures with Data Mining of Quantum Calculations. Physical Review Letters, 2003, 91, 135503.	7.8	354
15	SISSO: A compressed-sensing method for identifying the best low-dimensional descriptor in an immensity of offered candidates. Physical Review Materials, 2018, 2, .	2.4	349
16	Accuracy of ab initio methods in predicting the crystal structures of metals: A review of 80 binary alloys. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2005, 29, 163-211.	1.6	313
17	Machine learning modeling of superconducting critical temperature. Npj Computational Materials, 2018, 4, .	8.7	274
18	A search model for topological insulators with high-throughput robustness descriptors. Nature Materials, 2012, 11, 614-619.	27.5	244

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19	The AFLOW standard for high-throughput materials science calculations. Computational Materials Science, 2015, 108, 233-238.	3.0	244
20	Uptake of gases in bundles of carbon nanotubes. Physical Review B, 2000, 62, 2173-2180.	3.2	243
21	The 2019 materials by design roadmap. Journal Physics D: Applied Physics, 2019, 52, 013001.	2.8	236
22	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
23	Low thermal conductivity and triaxial phononic anisotropy of SnSe. Applied Physics Letters, 2014, 105, .	3.3	226
24	Dysprosium-doped cadmium oxide as a gateway material for mid-infrared plasmonics. Nature Materials, 2015, 14, 414-420.	27.5	216
25	High-Throughput Combinatorial Database of Electronic Band Structures for Inorganic Scintillator Materials. ACS Combinatorial Science, 2011, 13, 382-390.	3.8	211
26	Finding Unprecedentedly Low-Thermal-Conductivity Half-Heusler Semiconductors via High-Throughput Materials Modeling. Physical Review X, 2014, 4, .	8.9	210
27	Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints. Chemistry of Materials, 2015, 27, 735-743.	6.7	209
28	Machine learning for alloys. Nature Reviews Materials, 2021, 6, 730-755.	48.7	202
29	Accelerated discovery of new magnets in the Heusler alloy family. Science Advances, 2017, 3, e1602241.	10.3	197
30	Theoretical prediction of high melting temperature for a MoRuTaW HCP multiprincipal element alloy. Npj Computational Materials, 2021, 7, .	8.7	186
31	On-the-fly closed-loop materials discovery via Bayesian active learning. Nature Communications, 2020, 11, 5966.	12.8	167
32	A RESTful API for exchanging materials data in the AFLOWLIB.org consortium. Computational Materials Science, 2014, 93, 178-192.	3.0	148
33	The AFLOW Library of Crystallographic Prototypes: Part 1. Computational Materials Science, 2017, 136, S1-S828.	3.0	147
34	The search for high entropy alloys: A high-throughput ab-initio approach. Acta Materialia, 2018, 159, 364-383.	7.9	142
35	Discovery of high-entropy ceramics via machine learning. Npj Computational Materials, 2020, 6, .	8.7	133
36	Reformulation of $\langle \text{DFT} + \text{U} \rangle$ as a Pseudohybrid Hubbard Density Functional for Accelerated Materials Discovery. Physical Review X, 2015, 5, .	8.9	127

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37	Nanograined Half-Heusler Semiconductors as Advanced Thermoelectrics: An Ab Initio High-Throughput Statistical Study. <i>Advanced Functional Materials</i> , 2014, 24, 7427-7432.	14.9	117
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	How Chemical Composition Alone Can Predict Vibrational Free Energies and Entropies of Solids. <i>Chemistry of Materials</i> , 2017, 29, 6220-6227.	6.7	103
40	Hafnium binary alloys from experiments and first principles. <i>Acta Materialia</i> , 2010, 58, 2887-2897.	7.9	102
41	High-throughput and data mining with ab initio methods. <i>Measurement Science and Technology</i> , 2005, 16, 296-301.	2.6	100
42	Modeling the melting of supported clusters. <i>Applied Physics Letters</i> , 2006, 88, 133110.	3.3	95
43	Assessing the Thermoelectric Properties of Sintered Compounds via High-Throughput Ab-Initio Calculations. <i>Physical Review X</i> , 2011, 1, .	8.9	92
44	Thermopower of Molecular Junctions: An ab Initio Study. <i>Nano Letters</i> , 2009, 9, 1011-1014.	9.1	91
45	Decoupling Local Disorder and Optical Effects in Infrared Spectra: Differentiating Between Calcites with Different Origins. <i>Advanced Materials</i> , 2011, 23, 550-554.	21.0	91
46	Theoretical study of metal borides stability. <i>Physical Review B</i> , 2006, 74, .	3.2	79
47	Modeling Off-Stoichiometry Materials with a High-Throughput Ab-Initio Approach. <i>Chemistry of Materials</i> , 2016, 28, 6484-6492.	6.7	78
48	Prediction of different crystal structure phases in metal borides: A lithium monoboride analog to MgB <sub>2</sub> . <i>Physical Review B</i> , 2006, 73, .	3.2	77
49	PAOFLOW: A utility to construct and operate on ab initio Hamiltonians from the projections of electronic wavefunctions on atomic orbital bases, including characterization of topological materials. <i>Computational Materials Science</i> , 2018, 143, 462-472.	3.0	74
50	Predicting superhard materials via a machine learning informed evolutionary structure search. <i>Npj Computational Materials</i> , 2019, 5, .	8.7	74
51	Theoretical study of the thermal behavior of free and alumina-supported Fe-C nanoparticles. <i>Physical Review B</i> , 2007, 75, .	3.2	73
52	Reduced Carbon Solubility in Fe Nanoclusters and Implications for the Growth of Single-Walled Carbon Nanotubes. <i>Physical Review Letters</i> , 2008, 100, 195502.	7.8	73
53	AFLOW-ML: A RESTful API for machine-learning predictions of materials properties. <i>Computational Materials Science</i> , 2018, 152, 134-145.	3.0	72
54	A computational high-throughput search for new ternary superalloys. <i>Acta Materialia</i> , 2017, 122, 438-447.	7.9	70

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55	The AFLOW Library of Crystallographic Prototypes: Part 2. Computational Materials Science, 2019, 161, S1-S1011.	3.0	70
56	AFLOW <sup>W</sup> : 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
57	AFLOW-CHULL: Cloud-Oriented Platform for Autonomous Phase Stability Analysis. Journal of Chemical Information and Modeling, 2018, 58, 2477-2490.	5.4	69
58	Uncovering Compounds by Synergy of Cluster Expansion and High-Throughput Methods. Journal of the American Chemical Society, 2010, 132, 4830-4833.	13.7	68
59	An efficient and accurate framework for calculating lattice thermal conductivity of solids: AFLOW <sup>W</sup> APL Automatic Anharmonic Phonon Library. Npj Computational Materials, 2017, 3, .	8.7	65
60	The New Face of Rhodium Alloys: Revealing Ordered Structures from First Principles. Journal of the American Chemical Society, 2010, 132, 833-837.	13.7	64
61	Effective and accurate representation of extended Bloch states on finite Hilbert spaces. Physical Review B, 2013, 88, .	3.2	64
62	Crystallization behavior upon heating and cooling in Cu <sub>50</sub> Zr <sub>50</sub> metallic glass thin films. Acta Materialia, 2016, 121, 68-77.	7.9	64
63	Dynamics of an Inhomogeneously Coarse Grained Multiscale System. Physical Review Letters, 2002, 88, 255504.	7.8	62
64	Ordered Structures in Rhenium Binary Alloys from First-Principles Calculations. Journal of the American Chemical Society, 2011, 133, 158-163.	13.7	62
65	High-Throughput Computation of Thermal Conductivity of High-Temperature Solid Phases: The Case of Oxide and Fluoride Perovskites. Physical Review X, 2016, 6, .	8.9	61
66	Unavoidable disorder and entropy in multi-component systems. Npj Computational Materials, 2019, 5, .	8.7	61
67	Revealing the Impact of Catalyst Phase Transition on Carbon Nanotube Growth by <i>in Situ</i> Raman Spectroscopy. ACS Nano, 2013, 7, 1100-1107.	14.6	60
68	Hidden features of the catalyst nanoparticles favorable for single-walled carbon nanotube growth. Applied Physics Letters, 2007, 90, 163120.	3.3	59
69	Comparative Study of Nonproportionality and Electronic Band Structures Features in Scintillator Materials. IEEE Transactions on Nuclear Science, 2009, 56, 2989-2996.	2.0	59
70	Challenges in Ceramic Science: A Report from the Workshop on Emerging Research Areas in Ceramic Science. Journal of the American Ceramic Society, 2012, 95, 3699-3712.	3.8	59
71	Improved predictions of the physical properties of Zn- and Cd-based wide band-gap semiconductors: A validation of the ACBNO functional. Physical Review B, 2015, 91, .	3.2	56
72	AFLUX: The LUX materials search API for the AFLOW data repositories. Computational Materials Science, 2017, 137, 362-370.	3.0	56



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91	Accurate tight-binding Hamiltonians for two-dimensional and layered materials. <i>Physical Review B</i> , 2016, 93, .	3.2	40
92	High throughput combinatorial method for fast and robust prediction of lattice thermal conductivity. <i>Scripta Materialia</i> , 2017, 129, 88-93.	5.2	40
93	Coordination corrected ab initio formation enthalpies. <i>Npj Computational Materials</i> , 2019, 5, .	8.7	38
94	Entropy Landscaping of High-Entropy Carbides. <i>Advanced Materials</i> , 2021, 33, e2102904.	21.0	38
95	Computational Studies of Catalytic Particles for Carbon Nanotube Growth. <i>Journal of Computational and Theoretical Nanoscience</i> , 2009, 6, 1-15.	0.4	37
96	XtalOpt Version r12: An open-source evolutionary algorithm for crystal structure prediction. <i>Computer Physics Communications</i> , 2019, 237, 274-275.	7.5	37
97	Size dependent melting mechanisms of iron nanoclusters. <i>Chemical Physics</i> , 2007, 333, 57-62.	1.9	36
98	Search for high-T <sub>c</sub> in layered structures: The case of LiB. <i>Physical Review B</i> , 2007, 75, .	3.2	35
99	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
100	Data-Driven Quest for Two-Dimensional Non-van der Waals Materials. <i>Nano Letters</i> , 2022, 22, 989-997.	9.1	35
101	Ordered magnesium-lithium alloys: First-principles predictions. <i>Physical Review B</i> , 2010, 81, .	3.2	33
102	Computer simulations of the wetting properties of neon on heterogeneous surfaces. <i>Physical Review E</i> , 1999, 59, 4402-4407.	2.1	30
103	Giant spin Hall effect in two-dimensional monochalcogenides. <i>2D Materials</i> , 2019, 6, 025012.	4.4	30
104	Thermodynamic stabilities of ternary metal borides: An ab initio guide for synthesizing layered superconductors. <i>Physical Review B</i> , 2008, 78, .	3.2	29
105	AFLOW-XtalFinder: a reliable choice to identify crystalline prototypes. <i>Npj Computational Materials</i> , 2021, 7, .	8.7	28
106	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
107	Improved electronic structure and magnetic exchange interactions in transition metal oxides. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 444003.	1.8	28
108	Evidence Concerning Drying Behavior of Ne near a Cs Surface. <i>Physical Review Letters</i> , 2001, 87, 206103.	7.8	27

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109	Viscous State Effect on the Activity of Fe Nanocatalysts. ACS Nano, 2010, 4, 6950-6956.	14.6	27
110	Systematic Band Gap Tuning of BaSnO <sub>3</sub> via Chemical Substitutions: The Role of Clustering in Mixed-Valence Perovskites. Chemistry of Materials, 2017, 29, 9378-9385.	6.7	27
111	Spin Hall effect in prototype Rashba ferroelectrics GeTe and SnTe. Npj Computational Materials, 2020, 6, .	8.7	26
112	High-entropy ceramics: Propelling applications through disorder. MRS Bulletin, 2022, 47, 194-202.	3.5	26
113	Accurate <i>ab initio</i> tight-binding Hamiltonians: Effective tools for electronic transport and optical spectroscopy from first principles. Physical Review B, 2016, 94, .	3.2	25
114	Metallic glasses for biodegradable implants. Acta Materialia, 2019, 176, 297-305.	7.9	25
115	Influence of Mo on the Fe:Mo:C nanocatalyst thermodynamics for single-walled carbon nanotube growth. Physical Review B, 2008, 78, .	3.2	24
116	Predictions of the Pt <sub>8</sub> Ti Phase in Unexpected Systems. Journal of the American Chemical Society, 2010, 132, 6851-6854.	13.7	24
117	Ultrathin SnTe films as a route towards all-in-one spintronics devices. 2D Materials, 2020, 7, 025026.	4.4	24
118	First principles study of Ag, Au, and Cu surface segregation in FePt-L10. Applied Physics Letters, 2010, 97, 221908.	3.3	23
119	Calculation of solubility in titanium alloys from first principles. Acta Materialia, 2009, 57, 5314-5323.	7.9	21
120	Advanced modeling of materials with PAOFLOW 2.0: New features and software design. Computational Materials Science, 2021, 200, 110828.	3.0	21
121	Xe films on a decagonal Al-Ni-Co quasicrystalline surface. Physical Review B, 2006, 74, .	3.2	19
122	First-principles solubilities of alkali and alkaline-earth metals in Mg-B alloys. Physical Review B, 2009, 79, .	3.2	19
123	<i>Ground-state characterizations of systems predicted to exhibit</i> $L_{19}$ structures. Physical Review B, 2012, 85, .	3.2	19
124	Enhancing ductility in bulk metallic glasses by straining during cooling. Communications Materials, 2021, 2, .	6.9	16
125	The AFLOW Library of Crystallographic Prototypes: Part 3. Computational Materials Science, 2021, 199, 110450.	3.0	16
126	Wetting transition behavior of Xe on Cs and Cs-graphite. Physical Review B, 2004, 70, .	3.2	15



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127	Nonproportionality and Scintillation Studies of $\text{Eu}^{2+}\text{Sr}_{1-x}\text{Ca}_x\text{Si}_2\text{O}_7$ From 295 to 5 K. IEEE Transactions on Nuclear Science, 2012, 59, 2052-2056.	2.0	15
128	Accelerating disorder-order transitions of FePt by preforming a metastable AgPt phase. Acta Materialia, 2012, 60, 7258-7264.	7.9	15
129	Stable ordered structures of binary technetium alloys from first principles. Physical Review B, 2012, 85, .	3.2	14
130	Vibrational Properties of Metastable Polymorph Structures by Machine Learning. Journal of Chemical Information and Modeling, 2018, 58, 2460-2466.	5.4	14
131	Revealing low-temperature atomic ordering in bulk Co-Pt with the high-throughput ab-initio method. Applied Physics Letters, 2011, 99, 261902.	3.3	13
132	First principles thermodynamical modeling of the binodal and spinodal curves in lead chalcogenides. Physical Chemistry Chemical Physics, 2016, 18, 5005-5011.	2.8	13
133	Parametrically constrained geometry relaxations for high-throughput materials science. Npj Computational Materials, 2019, 5, .	8.7	13
134	Characterization of light output and scintillation emission in CsI(Tl), NaI(Tl), and $\text{LaBr}_3(\text{Ce})$ under isostatic pressure. Radiation Measurements, 2013, 56, 70-75.	1.4	11
135	Molybdenum-titanium phase diagram evaluated from <i>ab initio</i> calculations. Physical Review Materials, 2017, 1, .	2.4	11
136	Computational study of the thermal behavior of iron clusters on a porous substrate. Physical Review B, 2008, 77, .	3.2	10
137	Modeling the Thermoelectric Properties of $\text{Ti}_5\text{O}_9$ Magn $\text{Al}$ Phase Ceramics. Journal of Electronic Materials, 2016, 45, 5526-5532.	2.2	9
138	The Maximum Edge Weight Clique Problem: Formulations and Solution Approaches. Springer Optimization and Its Applications, 2017, , 217-237.	0.9	9
139	The AFLOW Fleet for Materials Discovery. , 2018, , 1-28.		9
140	Thermoelectric Properties of Minerals with the Mawsonite Structure. ACS Applied Energy Materials, 2019, 2, 8068-8078.	5.1	9
141	Mechanical Properties of Chemically Modified Clay. Scientific Reports, 2019, 9, 13698.	3.3	9
142	Vibrational spectral fingerprinting for chemical recognition of biominerals. ChemPhysChem, 2020, 21, 770-778.	2.1	9
143	Automated coordination corrected enthalpies with AFLOW-CCE. Physical Review Materials, 2021, 5, .	2.4	9
144	Structures and Topological Transitions of Hydrocarbon Films on Quasicrystalline Surfaces. Physical Review Letters, 2009, 102, 055501.	7.8	8

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145	Spinodal Superlattices of Topological Insulators. <i>Chemistry of Materials</i> , 2018, 30, 2331-2340.	6.7	8
146	AFLOW-QHA3P: Robust and automated method to compute thermodynamic properties of solids. <i>Physical Review Materials</i> , 2019, 3, .	2.4	8
147	High-throughput study of the static dielectric constant at high temperatures in oxide and fluoride cubic perovskites. <i>Physical Review Materials</i> , 2020, 4, .	2.4	8
148	Tin-pest problem as a test of density functionals using high-throughput calculations. <i>Physical Review Materials</i> , 2021, 5, .	2.4	7
149	The effect of lattice stability determination on the computational phase diagrams of intermetallic alloys. <i>Journal of Alloys and Compounds</i> , 2017, 728, 314-321.	5.5	6
150	Physics in the Machine: Integrating Physical Knowledge in Autonomous Phase-Mapping. <i>Frontiers in Physics</i> , 2022, 10, .	2.1	6
151	Thermodynamics of carbon in iron nanoparticles at low temperature: Reduced solubility and size-induced nucleation of cementite. <i>Physics Procedia</i> , 2010, 6, 16-26.	1.2	5
152	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
153	The Structure and Composition Statistics of 6A Binary and Ternary Crystalline Materials. <i>Inorganic Chemistry</i> , 2018, 57, 653-667.	4.0	4
154	The AFLOW Fleet for Materials Discovery. , 2020, , 1785-1812.		4
155	Data Mining Approach to Ab-Initio Prediction of Crystal Structure. <i>Materials Research Society Symposia Proceedings</i> , 2003, 804, 305.	0.1	3
156	Nonproportionality and Scintillation Responses of LSO:Ce From 4.3 to 300 K. <i>IEEE Transactions on Nuclear Science</i> , 2013, 60, 993-999.	2.0	3
157	The Microscopic Diamond Anvil Cell: Stabilization of Superhard, Superconducting Carbon Allotropes at Ambient Pressure. <i>Angewandte Chemie</i> , 2022, 134, .	2.0	3
158	Computational Studies of Small Carbon and Iron-Carbon Systems Relevant to Carbon Nanotube Growth. <i>Journal of Nanoscience and Nanotechnology</i> , 2008, 8, 6170-6177.	0.9	2
159	Networks of materials: Construction and structural analysis. <i>AIChE Journal</i> , 2021, 67, e17051.	3.6	2
160	Two-Layer High-Throughput: Effective Mass Calculations Including Warping. <i>Engineering</i> , 2022, 10, 74-80.	6.7	2
161	Lossless tapers, Gaussian beams, free-space modes: Standing waves versus through-flowing waves. <i>Optical and Quantum Electronics</i> , 2000, 32, 1161-1173.	3.3	1
162	Density functional study of the L10â€œIrV transition in IrV and RhV. <i>Journal of Alloys and Compounds</i> , 2011, 509, 560-567.	5.5	1

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163	Gasâ€œSurface Interactions on Quasicrystals. Israel Journal of Chemistry, 2011, 51, 1304-1313.	2.3	1
164	Numerical Algorithm for PÃ³lya Enumeration Theorem. Journal of Experimental Algorithmics, 2016, 21, 1-17.	1.0	1
165	First Principles Investigation of Cold Curves of Metals. Israel Journal of Chemistry, 2020, 60, 897-904.	2.3	1
166	High-Throughput Computational Search for Half-Metallic Oxides. Molecules, 2020, 25, 2010.	3.8	1
167	<title>Lossless tapers, Gaussian beams, and free-space modes: standing waves versus through-flowing waves</title>. , 1999, 3666, 199.		0
168	Dynamics and Thermodynamics of a system with multiple length scales. Materials Research Society Symposia Proceedings, 2002, 731, 441.	0.1	0
169	The AFLOW Fleet for Materials Discovery. , 2019, , 1-28.		0