# 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 | Data-Driven Quest for Two-Dimensional Non-van der Waals Materials. Nano Letters, 2022, 22, 989-997. | 9.1 | 35 |
| 2 | Physics in the Machine: Integrating Physical Knowledge in Autonomous Phase-Mapping. Frontiers in Physics, 2022, 10, . | 2.1 | 6 |
| 3 | Two-Layer High-Throughput: Effective Mass Calculations Including Warping. Engineering, 2022, 10, 74-80. | 6.7 | 2 |
| 4 | High-entropy ceramics: Propelling applications through disorder. MRS Bulletin, 2022, 47, 194-202. | 3.5 | 26 |
| 5 | The Microscopic Diamond Anvil Cell: Stabilization of Superhard, Superconducting Carbon Allotropes at Ambient Pressure. Angewandte Chemie - International Edition, 2022, 61, . | 13.8 | 5 |
| 6 | The Microscopic Diamond Anvil Cell: Stabilization of Superhard, Superconducting Carbon Allotropes at Ambient Pressure. Angewandte Chemie, 2022, 134, . | 2.0 | 3 |
| 7 | Networks of materials: Construction and structural analysis. AICHE Journal, 2021, 67, e17051. | 3.6 | 2 |
| 8 | Theoretical prediction of high melting temperature for a Moâ€“Ruâ€“Taâ€“W HCP multiprincipal element alloy. Npj Computational Materials, 2021, 7, . | 8.7 | 186 |
| 9 | AFLOW-XtalFinder: a reliable choice to identify crystalline prototypes. Npj Computational Materials, 2021, 7, . | 8.7 | 28 |
| 10 | Enhancing ductility in bulk metallic glasses by straining during cooling. Communications Materials, 2021, 2, . | 6.9 | 16 |
| 11 | Automated coordination corrected enthalpies with AFLOW-CCE. Physical Review Materials, 2021, 5, . | 2.4 | 9 |
| 12 | Machine learning for alloys. Nature Reviews Materials, 2021, 6, 730-755. | 48.7 | 202 |
| 13 | OPTIMADE, an API for exchanging materials data. Scientific Data, 2021, 8, 217. | 5.3 | 49 |
| 14 | Tin-pest problem as a test of density functionals using high-throughput calculations. Physical Review Materials, 2021, 5, . | 2.4 | 7 |
| 15 | Entropy Landscaping of Highâ€Entropy Carbides. Advanced Materials, 2021, 33, e2102904. | 21.0 | 38 |
| 16 | Settling the matter of the role of vibrations in the stability of high-entropy carbides. Nature Communications, 2021, 12, 5747. | 12.8 | 28 |
| 17 | The AFLOW Library of Crystallographic Prototypes: Part 3. Computational Materials Science, 2021, 199, 110450. | 3.0 | 16 |
| 18 | Advanced modeling of materials with PAOFLOW 2.0: New features and software design. Computational Materials Science, 2021, 200, 110828. | 3.0 | 21 |

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| 19 | On-the-fly closed-loop materials discovery via Bayesian active learning. Nature Communications, 2020, 11, 5966. | 12.8 | 167 |
| 20 | Vibrational spectral fingerprinting for chemical recognition of biominerals. ChemPhysChem, 2020, 21, 770-778. | 2.1 | 9 |
| 21 | Spin Hall effect in prototype Rashba ferroelectrics GeTe and SnTe. Npj Computational Materials, 2020, 6, . | 8.7 | 26 |
| 22 | First Principles Investigation of Cold Curves of Metals. Israel Journal of Chemistry, 2020, 60, 897-904. | 2.3 | 1 |
| 23 | High-entropy ceramics. Nature Reviews Materials, 2020, 5, 295-309. | 48.7 | 902 |
| 24 | Ultrathin SnTe films as a route towards all-in-one spintronics devices. 2D Materials, 2020, 7, 025026. | 4.4 | 24 |
| 25 | High-Throughput Computational Search for Half-Metallic Oxides. Molecules, 2020, 25, 2010. | 3.8 | 1 |
| 26 | Discovery of high-entropy ceramics via machine learning. Npj Computational Materials, 2020, 6, . | 8.7 | 133 |
| 27 | QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564. | 38.1 | 427 |
| 28 | High-throughput study of the static dielectric constant at high temperatures in oxide and fluoride cubic perovskites. Physical Review Materials, 2020, 4, . | 2.4 | 8 |
| 29 | The AFLOW Fleet for Materials Discovery. , 2020, , 1785-1812. | | 4 |
| 30 | The 2019 materials by design roadmap. Journal Physics D: Applied Physics, 2019, 52, 013001. | 2.8 | 236 |
| 31 | Unavoidable disorder and entropy in multi-component systems. Npj Computational Materials, 2019, 5, . | 8.7 | 61 |
| 32 | Metallic glasses for biodegradable implants. Acta Materialia, 2019, 176, 297-305. | 7.9 | 25 |
| 33 | Thermoelectric Properties of Minerals with the Mawsonite Structure. ACS Applied Energy Materials, 2019, 2, 8068-8078. | 5.1 | 9 |
| 34 | Predicting superhard materials via a machine learning informed evolutionary structure search. Npj Computational Materials, 2019, 5, . | 8.7 | 74 |
| 35 | Mechanical Properties of Chemically Modified Clay. Scientific Reports, 2019, 9, 13698. | 3.3 | 9 |
| 36 | The AFLOW Library of Crystallographic Prototypes: Part 2. Computational Materials Science, 2019, 161, S1-S1011. | 3.0 | 70 |

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| 37 | Coordination corrected ab initio formation enthalpies. Npj Computational Materials, 2019, 5, . | 8.7 | 38 |
| 38 | Giant spin Hall effect in two-dimensional monochalcogenides. 2D Materials, 2019, 6, 025012. | 4.4 | 30 |
| 39 | The AFLOW Fleet for Materials Discovery. , 2019, , 1-28. | | 0 |
| 40 | Parametrically constrained geometry relaxations for high-throughput materials science. Npj Computational Materials, 2019, 5, . | 8.7 | 13 |
| 41 | Phase stability and mechanical properties of novel high entropy transition metal carbides. Acta Materialia, 2019, 166, 271-280. | 7.9 | 422 |
| 42 | XtalOptÂVersion r12: An open-source evolutionary algorithm for crystal structure prediction. Computer Physics Communications, 2019, 237, 274-275. | 7.5 | 37 |
| 43 | AFLOW-QHA3P: Robust and automated method to compute thermodynamic properties of solids. Physical Review Materials, 2019, 3, . | 2.4 | 8 |
| 44 | The Structure and Composition Statistics of 6A Binary and Ternary Crystalline Materials. Inorganic Chemistry, 2018, 57, 653-667. | 4.0 | 4 |
| 45 | AFLOW-SYM: 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 |
| 46 | Spinodal Superlattices of Topological Insulators. Chemistry of Materials, 2018, 30, 2331-2340. | 6.7 | 8 |
| 47 | 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. Computational Materials Science, 2018, 143, 462-472. | 3.0 | 74 |
| 48 | The AFLOW Fleet for Materials Discovery. , 2018, , 1-28. | | 9 |
| 49 | High-entropy high-hardness metal carbides discovered by entropy descriptors. Nature Communications, 2018, 9, 4980. | 12.8 | 604 |
| 50 | Vibrational Properties of Metastable Polymorph Structures by Machine Learning. Journal of Chemical Information and Modeling, 2018, 58, 2460-2466. | 5.4 | 14 |
| 51 | AFLOW-CHULL: Cloud-Oriented Platform for Autonomous Phase Stability Analysis. Journal of Chemical Information and Modeling, 2018, 58, 2477-2490. | 5.4 | 69 |
| 52 | Data-driven design of inorganic materials with the Automatic Flow Framework for Materials Discovery. MRS Bulletin, 2018, 43, 670-675. | 3.5 | 35 |
| 53 | AFLOW-ML: A RESTful API for machine-learning predictions of materials properties. Computational Materials Science, 2018, 152, 134-145. | 3.0 | 72 |
| 54 | The search for high entropy alloys: A high-throughput ab-initio approach. Acta Materialia, 2018, 159, 364-383. | 7.9 | 142 |

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| 55 | Machine learning modeling of superconducting critical temperature. Npj Computational Materials, 2018, 4, . | 8.7 | 274 |
| 56 | 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 |
| 57 | Accelerated discovery of new magnets in the Heusler alloy family. Science Advances, 2017, 3, e1602241. | 10.3 | 197 |
| 58 | How Chemical Composition Alone Can Predict Vibrational Free Energies and Entropies of Solids. Chemistry of Materials, 2017, 29, 6220-6227. | 6.7 | 103 |
| 59 | The AFLOW Library of Crystallographic Prototypes: Part 1. Computational Materials Science, 2017, 136, S1-S828. | 3.0 | 147 |
| 60 | An efficient and accurate framework for calculating lattice thermal conductivity of solids: AFLOWâ€"AAPL Automatic Anharmonic Phonon Library. Npj Computational Materials, 2017, 3, . | 8.7 | 65 |
| 61 | 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 |
| 62 | The effect of lattice stability determination on the computational phase diagrams of intermetallic alloys. Journal of Alloys and Compounds, 2017, 728, 314-321. | 5.5 | 6 |
| 63 | AFLUX: The LUX materials search API for the AFLOW data repositories. Computational Materials Science, 2017, 137, 362-370. | 3.0 | 56 |
| 64 | A computational high-throughput search for new ternary superalloys. Acta Materialia, 2017, 122, 438-447. | 7.9 | 70 |
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| 66 | Universal fragment descriptors for predicting properties of inorganic crystals. Nature Communications, 2017, 8, 15679. | 12.8 | 435 |
| 67 | The Maximum Edge Weight Clique Problem: Formulations and Solution Approaches. Springer Optimization and Its Applications, 2017, , 217-237. | 0.9 | 9 |
| 68 | 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 |
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| 70 | Combining the AFLOW GIBBS and elastic libraries to efficiently and robustly screen thermomechanical properties of solids. Physical Review Materials, 2017, 1, . | 2.4 | 47 |
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| 75 | Numerical Algorithm for PÃ³lya Enumeration Theorem. Journal of Experimental Algorithmics, 2016, 21, 1-17. | 1.0 | 1 |
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| 77 | Modeling Off-Stoichiometry Materials with a High-Throughput Ab-Initio Approach. Chemistry of Materials, 2016, 28, 6484-6492. | 6.7 | 78 |
| 78 | Crystallization behavior upon heating and cooling in Cu50Zr50 metallic glass thin films. Acta Materialia, 2016, 121, 68-77. | 7.9 | 64 |
| 79 | Accurate tight-binding Hamiltonian matrices fromab initiocalculations: Minimal basis sets. Physical Review B, 2016, 93, . | 3.2 | 43 |
| 80 | Accurate tight-binding Hamiltonians for two-dimensional and layered materials. Physical Review B, 2016, 93, . | 3.2 | 40 |
| 81 | Spectral descriptors for bulk metallic glasses based on the thermodynamics of competing crystalline phases. Nature Communications, 2016, 7, 12315. | 12.8 | 104 |
| 82 | Accurateab initiotight-binding Hamiltonians: Effective tools for electronic transport and optical spectroscopy from first principles. Physical Review B, 2016, 94, . | 3.2 | 25 |
| 83 | First principles thermodynamical modeling of the binodal and spinodal curves in lead chalcogenides. Physical Chemistry Chemical Physics, 2016, 18, 5005-5011. | 2.8 | 13 |
| 84 | The AFLOW standard for high-throughput materials science calculations. Computational Materials Science, 2015, 108, 233-238. | 3.0 | 244 |
| 85 | Finding the stable structures of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mtext>N</mml:mtext><mml:mrow><mml:mn> anab initiohigh-throughput approach. Physical Review B, 2015, 91, . | 3.2 | 54 |
| 86 | Improved predictions of the physical properties of Zn- and Cd-based wide band-gap semiconductors: A validation of the ACBN0 functional. Physical Review B, 2015, 91, . | 3.2 | 56 |
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| 88 | Dysprosium-doped cadmium oxide as a gateway material for mid-infrared plasmonics. Nature Materials, 2015, 14, 414-420. | 27.5 | 216 |
| 89 | Reformulation of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>DFT</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math>as a Pseudohybrid Hubbard Density Functional for Accelerated Materials Discovery. Physical Review X, 2015, 5, . | 8.9 | 127 |
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| 92 | Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints. Chemistry of Materials, 2015, 27, 735-743. | 6.7 | 209 |
| 93 | Robust topological surface state in Kondo insulator SmB<sub>6</sub> thin films. Applied Physics Letters, 2014, 105, 222403. | 3.3 | 42 |
| 94 | Finding Unprecedentedly Low-Thermal-Conductivity Half-Heusler Semiconductors via High-Throughput Materials Modeling. Physical Review X, 2014, 4, . | 8.9 | 210 |
| 95 | High-throughput computational screening of thermal conductivity, Debye temperature, and GrÃ¼neisen parameter using a quasiharmonic Debye model. Physical Review B, 2014, 90, . | 3.2 | 230 |
| 96 | A RESTful API for exchanging materials data in the AFLOWLIB.org consortium. Computational Materials Science, 2014, 93, 178-192. | 3.0 | 148 |
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| 98 | Low thermal conductivity and triaxial phononic anisotropy of SnSe. Applied Physics Letters, 2014, 105, . | 3.3 | 226 |
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| 103 | The high-throughput highway to computational materials design. Nature Materials, 2013, 12, 191-201. | 27.5 | 1,475 |
| 104 | Revealing the Impact of Catalyst Phase Transition on Carbon Nanotube Growth byin SituRaman Spectroscopy. ACS Nano, 2013, 7, 1100-1107. | 14.6 | 60 |
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| 106 | Stable ordered structures of binary technetium alloys from first principles. Physical Review B, 2012, 85, . | 3.2 | 14 |
| 107 | Ground-state characterizations of systems predicted to exhibit<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>L</mml:mi><mml:msub><mml:mn>1</mml:mn><mml:mn>1</mml:mn></mml:msub></mml:mrow></mml:math>structures. Physical Review B, 2012, 85, . | 3.2 | 19 |
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| 109 | AFLOW: An automatic framework for high-throughput materials discovery. Computational Materials Science, 2012, 58, 218-226. | 3.0 | 898 |
| 110 | AFLOWLIB.ORG: A distributed materials properties repository from high-throughput ab initio calculations. Computational Materials Science, 2012, 58, 227-235. | 3.0 | 811 |
| 111 | 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 |
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| 117 | High-Throughput Combinatorial Database of Electronic Band Structures for Inorganic Scintillator Materials. ACS Combinatorial Science, 2011, 13, 382-390. | 3.8 | 211 |
| 118 | Assessing the Thermoelectric Properties of Sintered Compounds via High-ThroughputAb-InitioCalculations. Physical Review X, 2011, 1, . | 8.9 | 92 |
| 119 | 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 |
| 120 | Density functional study of the L10â€“Î±IrV transition in IrV and RhV. Journal of Alloys and Compounds, 2011, 509, 560-567. | 5.5 | 1 |
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| 124 | Surface segregation in nanoparticles from first principles: The case of FePt. Scripta Materialia, 2010, 62, 179-182. | 5.2 | 49 |
| 125 | Thermodynamics of carbon in iron nanoparticles at low temperature: Reduced solubility and size-induced nucleation of cementite. Physics Procedia, 2010, 6, 16-26. | 1.2 | 5 |
| 126 | Hafnium binary alloys from experiments and first principles. Acta Materialia, 2010, 58, 2887-2897. | 7.9 | 102 |

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| 128 | 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 |
| 129 | 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 |
| 130 | Viscous State Effect on the Activity of Fe Nanocatalysts. ACS Nano, 2010, 4, 6950-6956. | 14.6 | 27 |
| 131 | Uncovering Compounds by Synergy of Cluster Expansion and High-Throughput Methods. Journal of the American Chemical Society, 2010, 132, 4830-4833. | 13.7 | 68 |
| 132 | High-throughput electronic band structure calculations: Challenges and tools. Computational Materials Science, 2010, 49, 299-312. | 3.0 | 1,140 |
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| 136 | Structures and Topological Transitions of Hydrocarbon Films on Quasicrystalline Surfaces. Physical Review Letters, 2009, 102, 055501. | 7.8 | 8 |
| 137 | Comparative Study of Nonproportionality and Electronic Band Structures Features in Scintillator Materials. IEEE Transactions on Nuclear Science, 2009, 56, 2989-2996. | 2.0 | 59 |
| 138 | Computational Studies of Catalytic Particles for Carbon Nanotube Growth. Journal of Computational and Theoretical Nanoscience, 2009, 6, 1-15. | 0.4 | 37 |
| 139 | Calculation of solubility in titanium alloys from first principles. Acta Materialia, 2009, 57, 5314-5323. | 7.9 | 21 |
| 140 | Thermopower of Molecular Junctions: An ab Initio Study. Nano Letters, 2009, 9, 1011-1014. | 9.1 | 91 |
| 141 | Reduced Carbon Solubility in Fe Nanoclusters and Implications for the Growth of Single-Walled Carbon Nanotubes. Physical Review Letters, 2008, 100, 195502. | 7.8 | 73 |
| 142 | Thermodynamic stabilities of ternary metal borides: Anab initioguide for synthesizing layered superconductors. Physical Review B, 2008, 78, . | 3.2 | 29 |
| 143 | Influence of Mo on the Fe:Mo:C nanocatalyst thermodynamics for single-walled carbon nanotube growth. Physical Review B, 2008, 78, . | 3.2 | 24 |
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| 155 | Evolution of Topological Order in Xe Films on a Quasicrystal Surface. Physical Review Letters, 2005, 95, 136104. | 7.8 | 40 |
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| 166 | Uptake of gases in bundles of carbon nanotubes. Physical Review B, 2000, 62, 2173-2180. | 3.2 | 243 |
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| 168 | Atoms in nanotubes: Small dimensions and variable dimensionality. American Journal of Physics, 1999, 67, 1170-1176. | 0.7 | 42 |
| 169 | <title>Lossless tapers, Gaussian beams, and free-space modes: standing waves versus through-flowing waves</title>. , 1999, 3666, 199. | | 0 |