

# COREY OSES

Materials Science, Duke University

Personal Information · Objective · Work Experience and Skills · Education · Press and News Releases · Honors and Awards · Workshops · Talks/Presentations · Journal Publications · Book Publications · Teaching Experience · Certifications · Activities and Outreach

## PERSONAL INFORMATION

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## OBJECTIVE

To obtain a graduate degree and perform research relevant to Materials Science and Engineering in order to develop my technical and managerial skills toward academia and make significant contributions to Duke University.

## WORK EXPERIENCE AND SKILLS

<i>Proficient Coder</i>	Present	C++, Python, $\text{\LaTeX}$ , MATLAB & R
<i>Postdoctoral Fellow</i>	2018–present	Duke University <b>Supervisor:</b> S. Curtarolo
<i>Internship</i>	Summer 2013	Cornell High Energy Synchrotron Source (BioSAXS on F2 and G Beamlines) Developed software for analyzing proteins with SAXS (small angle X-Ray scattering) measurements (Guinier plots). <b>Supervisors:</b> R. E. Gillilan & E. Fontes
<i>Internship</i>	Summer 2012	Cornell High Energy Synchrotron Source (Capillary Optics Group) Designed a beam stop assembly to eliminate parasitic X-Ray beams and improve focusing capabilities of the ellipsoidal glass capillary optic. <b>Supervisors:</b> R. Huang & E. Fontes
<i>Office Assistant</i>	Summer 2011	ILR Budget Office, Cornell University <b>Supervisor:</b> R. M. Cook
<i>Externship</i>	March 2010	Supreme Court of New York <b>Supervisors:</b> A. E. Belen & A. Hurkin-Torres
<i>Math Tutor</i>	Fall 2008	Graduate Record Exam (GRE)
<i>Office Assistant</i>	Summer 2008	SOS Security, LLC in Parsippany, NJ <b>Supervisor:</b> J. Flanagan

## EDUCATION

<i>Ph.D.</i>	2013–2018	Duke University <b>GPA:</b> 3.8/4.0 · <b>Department:</b> Mechanical Engineering and Materials Science <b>Thesis:</b> <i>Machine learning, phase stability, and disorder with the Automatic Flow Framework for Materials Discovery</i> <b>ProQuest:</b> <a href="http://search.proquest.com/docview/2172402640?pq-origsite=gscholar">search.proquest.com/docview/2172402640?pq-origsite=gscholar</a> <b>Advisor:</b> S. Curtarolo
<i>B.Sc.</i>	2009–2013	Cornell University <b>GPA:</b> 3.3/4.0 · <b>Department:</b> Applied and Engineering Physics <b>Thesis:</b> <i>Plume Propagation Simulation for Pulsed Laser Deposition</i> <b>Advisor:</b> J. Brock
<i>High School Diploma</i>	2005–2009	Bloomfield High School <b>GPA:</b> 3.9/4.0 · <i>Graduated fifth in class of 428</i>

## PRESS AND NEWS RELEASES

Duke University Pratt School of Engineering	November 2018	<p><i>"Disordered Materials Could Be Hardest, Most Heat-Tolerant Ever"</i></p> <ul style="list-style-type: none"> <li>This press release is featured on <a href="#">AAAS EurekAlert!</a>, <a href="#">Phys.org</a>, <a href="#">ScienceDaily</a>, <a href="#">Science Bulletin</a>, <a href="#">Naaju, NewsBeezer</a>, <a href="#">RemoNews</a>, <a href="#">Tech2</a>, and <a href="#">LongRoom News</a>.</li> </ul> <p><a href="http://pratt.duke.edu/about/news/chaotic-carbides">pratt.duke.edu/about/news/chaotic-carbides</a></p>
Diversity in Action	September 2018	<p><i>"Options in Education: Building Bridges — Pratt School of Engineering mentors underrepresented students"</i></p> <p><a href="http://bluetoad.com/publication/?i=521423&amp;ver=html5&amp;p=70#&amp;">bluetoad.com/publication/?i=521423&amp;ver=html5&amp;p=70#&amp;</a></p>
MRS Bulletin	August 2017	<p><i>"Universal fragment descriptor predicts materials properties"</i></p> <p><a href="http://cambridge.org/core/journals/mrs-bulletin/news/universal-fragment-descriptor-predicts-materials-properties">cambridge.org/core/journals/mrs-bulletin/news/universal-fragment-descriptor-predicts-materials-properties</a></p>
UNC Eshelman School of Pharmacy	June 2017	<p><i>"Breakthrough Tool Predicts Properties of Theoretical Materials, Finds New Uses for Current Ones"</i></p> <ul style="list-style-type: none"> <li>This press release is featured on <a href="#">AAAS EurekAlert!</a>, <a href="#">Phys.org</a>, and <a href="#">ScienceDaily</a>.</li> </ul> <p><a href="http://pharmacy.unc.edu/news/2017/06/06/breakthrough-tool-predicts-properties-theoretical-materials-finds-new-uses-current-ones/">pharmacy.unc.edu/news/2017/06/06/breakthrough-tool-predicts-properties-theoretical-materials-finds-new-uses-current-ones/</a></p>
Duke University Pratt School of Engineering	April 2017	<p><i>"Computers Create Recipe for Two New Magnetic Materials"</i></p> <ul style="list-style-type: none"> <li>This press release is featured on <a href="#">Phys.org</a>, <a href="#">Slashdot</a>, <a href="#">Hacker News</a>, <a href="#">Reddit</a>, <a href="#">Engadget</a>, <a href="#">Engineering.com</a>, <a href="#">Science Alert</a>, <a href="#">Azo Materials</a>, <a href="#">Next Big Future</a>, <a href="#">Futurism</a>, <a href="#">New Atlas</a>, and <a href="#">International Business Times</a>.</li> </ul> <p><a href="http://pratt.duke.edu/about/news/predicting-magnets">pratt.duke.edu/about/news/predicting-magnets</a></p>
MRS Bulletin	April 2015	<p><i>"Materials fingerprints identified for informatics"</i></p> <p><a href="https://doi.org/10.1557/mrs.2015.76">doi.org/10.1557/mrs.2015.76</a></p>
Computational Chemistry Highlights	January 2015	<p><i>"Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints"</i></p> <ul style="list-style-type: none"> <li>"This paper is a <a href="#">tour de force</a> for computational materials science" — Prof. Aspuru-Guzik.</li> </ul> <p><a href="http://compchemhighlights.org/2015/01/materials-cartography-representing-and.html">compchemhighlights.org/2015/01/materials-cartography-representing-and.html</a></p>
Duke University Research	January 2015	<p><i>"Molecular Tornado"</i></p> <p><a href="http://research.duke.edu/molecular-tornado">research.duke.edu/molecular-tornado</a></p>
Duke University Graduate School	October 2014	<p><i>"Competing for NSF Fellowships: Advice from a Current Fellow"</i></p> <p><a href="http://gradschool.duke.edu/professional-development/blog/competing-nsf-fellowships-advice-current-fellow">gradschool.duke.edu/professional-development/blog/competing-nsf-fellowships-advice-current-fellow</a></p>
Duke University Pratt School of Engineering	June 2014	<p><i>"Pratt Profiles: Corey Oses"</i></p> <p><a href="http://pratt.duke.edu/graduate/diversity/pratt-profiles-corey-oses">pratt.duke.edu/graduate/diversity/pratt-profiles-corey-oses</a></p>
Duke University MEM Program	November 2013	<p><i>"Society of Hispanic Professional Engineers"</i></p> <p><a href="http://memp.pratt.duke.edu/news/society-hispanic-professional-engineers">memp.pratt.duke.edu/news/society-hispanic-professional-engineers</a></p>
New York Kiwanis	February 2013	<p><i>"New York Kiwanis Mid-Winter Conference 2013"</i></p> <p><a href="http://kiwanis-ny.org/1213/midyear.htm">kiwanis-ny.org/1213/midyear.htm</a></p>
ERN Conference 2013	February 2013	<p><i>"2013 Oral and Poster Presentation Award Winners"</i></p> <p><a href="http://new.emerging-researchers.org/2013-oral-and-poster-presentation-winners">new.emerging-researchers.org/2013-oral-and-poster-presentation-winners</a></p>
New York Kiwanis	June 2012	<p><i>"K-Kids Show Talent for Fundraising"</i></p> <p><a href="http://patch.com/new-york/eastmeadow/k-kids-show-talent-for-fundraising">patch.com/new-york/eastmeadow/k-kids-show-talent-for-fundraising</a></p>
New York Kiwanis	March 2012	<p><i>"Past Circle K Governors Help Celebrate 50th Convention"</i></p> <p>Elected Governor of New York Circle K.</p> <p><a href="http://kiwanis-ny.org/news/view_news.php?nid=618">kiwanis-ny.org/news/view_news.php?nid=618</a></p>

## HONORS AND AWARDS

November 09, 2018	Presentation Finalist at the Engineering Science Symposium, SHPE National Conference
2018	Editor's Choice, Publication in Comput. Mater. Sci., Elsevier

November 03, 2017	Presentation Winner at the Engineering Science Symposium, SHPE National Conference
2017	Editor's Choice, Publication in Comput. Mater. Sci., Elsevier
November 04, 2016	Presentation Finalist at the Engineering Science Symposium, SHPE National Conference
August 14, 2015	Best Teaching Assistant Award (ME 221), Duke University Department of Mechanical Engineering and Materials Science
2015	Editor's Choice, Publication in Comput. Mater. Sci., Elsevier
2015	Editor's Choice, Publication in Chem. Mater., American Chemical Society
2013–2016	Graduate Research Fellowship, National Science Foundation
2013–2015	Associate Fellow, National GEM Consortium
November 01, 2013	Technical Poster and Paper Finalist at the Engineering Science Symposium, SHPE National Conference
August 22, 2013	Best Presentation Award at the MEMS Departmental Retreat, Duke University Department of Mechanical Engineering and Materials Science
March 21, 2013	New York City Citation as Circle K Governor, Council Member Fernando Cabrera
March 02, 2013	First Place in Nanoscience and Physics Research Presentation, NSF / AAAS / EHR Emerging Researchers National Conference
October 08, 2011	College Bowl Winner, Hispanic Engineer National Achievement Awards Conference (HENAAC)
Northrop Grumman One Team	
2011–2013	Shell Incentive Fund Scholarship
2010–2013	Louis Stokes Alliance for Minority Participation (LSAMP) Scholar
2010 & 2011	Xerox Corporation Scholarship
2010 & 2011	Intel Academic Award
2010–2013	GE Foundation / LULAC Scholarship
June 18, 2010	Cornell University Unmanned Air Systems Team awarded \$1,000 grant, AUVSI Student Unmanned Aerial Systems Competition
2009–2013	Meinig Family Cornell National Scholars
Awarded by Peter Meinig (Past Chairman of the Board of Trustees at Cornell University)	
2009	<i>Men of Principle</i> Award, Beta Theta Pi
Beta Delta Chapter	
2009	<a href="#">Gold Medallion Winner in Engineering and Mathematics</a> , Hispanic Heritage Youth Awards
2009	New Jersey Principals and Supervisors Association Scholarship
2009	Edward J. Bloustein Distinguished Scholar
2009	Investors Savings Bank Scholarship
2009	Bloomfield Education Association Scholarship
2009	Special Recognition Award, Bloomfield Kiwanis
2009	The Harold Brotherhood Award
2009	Jean Doswell Oakes Scholarship, Oakeside Cultural Center
2009	<a href="#">Superintendent's Bengal Pride Award</a> for Excellence in Academics and Citizenship
2009	<a href="#">Outstanding Student Citizen</a> for Youth Week, Bloomfield High School

2009	<a href="#">First Place Impromptu Essay</a> , New Jersey Key Club Convention
2009	Good Citizen Award, The Daughters of the American Revolution
2008–2009	National Honor Society
2008–2009	Scholar Athlete, Bloomfield High School
2006–2009	Academic Excellence, Bloomfield High School
2008	National Ventures Scholar Program
2008	Yale Book Club Award, Yale Club of Montclair, New Jersey

## WORKSHOPS

*AFLOW School: Integrated infrastructure for computational materials discovery*

**Co-Organizers:** C. Toher, D. Hicks, M. Esters, E. Gossett, R. Friedrich, M. J. Brenner & S. Curtarolo

8. **Presenter** at the Dresden Center for Computational Materials Science (DCMS) Materials 4.0 Summer School 2020, Technische Universität Dresden — August 18, 2020.
  - “Thermodynamics: AFLOW-CHULL” recording: [youtu.be/ncm356YNBVc](https://youtu.be/ncm356YNBVc)
7. **Presenter** at the NIST/Moore Foundation/University of Maryland Machine Learning for Materials Research Bootcamp 2019 & Workshop on Machine Learning Quantum Materials, Institute for Bioscience & Biotechnology Research in Gaithersburg, Maryland — July 23, 2020.
  - “Materials Database and Machine Learning: AFLOW-ML” recording: [youtu.be/x2qeBtOXues](https://youtu.be/x2qeBtOXues)
6. **Organizer and presenter** at the Texas A&M University AFLOW Multi-Day Workshop, College Station, Texas — June 16–18, 2020.
  - “Introduction to Density Functional Theory: VASP” recording: [youtu.be/ChySAfo2w7g](https://youtu.be/ChySAfo2w7g)
  - “Thermodynamics: AFLOW-CHULL” recording: [youtu.be/9Sa8D4inJ5w](https://youtu.be/9Sa8D4inJ5w)
  - “Disorder: AFLOW-POCC” recording: [youtu.be/xr-mU-1ShQQ](https://youtu.be/xr-mU-1ShQQ)
5. **Presenter** at the NIST/Moore Foundation/University of Maryland Machine Learning for Materials Research Bootcamp 2019 & Workshop on Machine Learning Quantum Materials, Institute for Bioscience & Biotechnology Research in Gaithersburg, Maryland — August 05, 2019.
4. **Organizer and presenter** at the University of Pennsylvania AFLOW Full-Day Workshop, Philadelphia, Pennsylvania — May 03, 2019.
3. **Organizer and presenter** at the North Carolina State University AFLOW Full-Day Workshop, Raleigh, North Carolina — March 12, 2019.
2. **Organizer and presenter** at the Carnegie Mellon University AFLOW Full-Day Workshop, Pittsburgh, Pennsylvania — January 21, 2019.
1. **Presenter** at the NIST/Moore Foundation/University of Maryland Machine Learning for Materials Research Bootcamp 2018 & Workshop on Machine Learning Quantum Materials, Institute for Bioscience & Biotechnology Research in Gaithersburg, Maryland — August 02, 2018.

## TALKS / PRESENTATIONS

*Entropy and ceramics: A valuable partnership*

31. **Invited seminar** at the Weizmann Institute of Science Department of Materials and Interfaces Seminar, Rehovot, Israel — February 06, 2020.
30. **Invited seminar** at the Tel Aviv University Sackler Center for Computational Molecular and Materials Science Seminar, Tel Aviv, Israel — February 05, 2020.
29. **Invited seminar** at the Ben-Gurion University of the Negev Materials Science Department Seminar, Beer Sheva, Israel — January 29, 2020.

*Cloud-oriented computational phase diagrams with AFLOW-CHULL*

28. **Contributed talk** at the American Physical Society March Meeting, Boston, Massachusetts — March 07, 2019.
27. **Poster presentation** at the CECAM (Centre Européen de Calcul Atomique et Moléculaire) Open Databases Integration for Materials Design (OPTiMaDe) Workshop, Lausanne, Switzerland — June 11, 2018.

*Going Off-Stoichiometry: Challenging Traditional Materials Discovery*

26. **Invited talk** at the Naval Research Laboratory Center for Computational Materials Science Seminar, Washington, D.C. — January 09, 2019.

*AFLOW-CHULL: Cloud-oriented platform for autonomous phase stability analysis*

25. **Contributed talk** at the SHPE National Conference, Cleveland, Ohio — November 09, 2018.
  - Presentation Finalist at the Engineering Science Symposium

*Machine learning, phase stability, and disorder with the Automatic Flow Framework for Materials Discovery*

24. **PhD defense** at the Duke University Ph.D. Thesis Defense, Durham, North Carolina — October 31, 2018.
  - Passed thesis defense
23. **PhD preliminary exam** at the Duke University Ph.D. Preliminary Exam, Durham, North Carolina — June 24, 2016.
  - Passed preliminary examination
22. **PhD qualifying exam** at the Duke University Ph.D. Qualifying Exam, Durham, North Carolina — August 07, 2014.
  - Passed qualifying examination
  - Subjects: Computational Materials Science, Statistical Mechanics, and Applied Partial Differential Equations and Complex Variables

*Universal Fragment Descriptors for Predicting Properties of Inorganic Crystals*

21. **Contributed talk** at the International Association for Computational Mechanics (IACM) 13<sup>th</sup> World Congress in Computational Mechanics (WCCM), New York City, New York — July 23, 2018.
20. **Contributed talk** at the Hopkins Extreme Materials Institute Mach Conference, Annapolis, Maryland — April 05, 2018.
19. **Contributed talk** at the SHPE National Conference, Kansas City, Missouri — November 03, 2017.
  - [Presentation Winner at the Engineering Science Symposium](#)
18. **Contributed talk** at the Duke University Chemistry Department Third Annual Graduate Research Symposium, Durham, North Carolina — October 09, 2017.
17. **Contributed talk** at the American Physical Society March Meeting, New Orleans, Louisiana — March 14, 2017.

*Advancements in Materials Informatics with AFLOW*

16. **Invited talk** at the Fritz-Haber-Institut der Max-Planck-Gesellschaft Theory Department Seminar, Berlin, Germany — January 18, 2018.
15. **Invited talk** at the Humboldt University of Berlin Physics Department Seminar, Berlin, Germany — January 16, 2018.

*Modeling Off-Stoichiometric Materials with a High-Throughput, Ab-Initio Approach*

14. **Contributed talk** at the SHPE National Conference, Seattle, Washington — November 04, 2016.
  - Presentation Finalist at the Engineering Science Symposium
13. **Contributed talk** at the American Physical Society March Meeting, Baltimore, Maryland — March 16, 2016.

*Materials Cartography: Representing and Mining Materials Space using Structural and Electronic Fingerprints*

12. **Invited talk** at the Brigham Young University Condensed Matter Physics Seminar, Provo, Utah — February 18, 2016.
11. **Contributed talk** at the Duke Mechanical Engineering and Materials Science (MEMS) Department Graduate Student Seminar, Durham, North Carolina — September 25, 2015.
10. **Contributed talk** at the American Physical Society March Meeting, San Antonio, Texas — March 02, 2015.

*Plume Propagation Simulation for Pulsed Laser Deposition*

9. **Poster presentation** at the University of Texas at Austin Machine Learning Summer School (MLSS), Austin, Texas — January 12, 2015.
8. **Contributed talk** at the NSF / AAAS / EHR Emerging Researchers National Conference, Washington, D.C. — February 22, 2014.
7. **Poster presentation** at the MRS / ASM / AVS / AReMS Meeting, North Carolina State University, Raleigh, North Carolina — November 15, 2013.
6. **Poster presentation** at the SHPE National Conference, Indianapolis, Indiana — November 01, 2013.
  - Technical Poster and Paper Finalist at the Engineering Science Symposium
5. **Poster presentation** at the Duke Mechanical Engineering and Materials Science (MEMS) Department Annual Retreat, Durham, North Carolina — August 22, 2013.
  - [Best Presentation Award](#)

*Synchrotron Radiation Focusing Optics — Capillary Beam Stop Design*

4. **Contributed talk** at the NSF / AAAS / EHR Emerging Researchers National Conference, Washington, D.C. — March 02, 2013.
  - [First Place in Nanoscience and Physics Research Presentation](#)
3. **Poster presentation** at the Cornell University Chapter of LSAMP Research Symposium, Ithaca, New York — August 07, 2012.

*AEOLUS Unmanned Aerial Reconnaissance System by CU AIR*

2. **Group presentation** at the Association for Unmanned Vehicle Systems International (AUVSI) Student Unmanned Aerial Systems Competition (SUAS), Patuxent River Naval Air Station, Maryland — June 24, 2010.
  - [Team awarded \\$1,000 grant](#)

*Academic Integrity*

1. **Group presentation** at the Meinig Family Cornell National Scholars Freshman Forum, Ithaca, New York — April 21, 2010.

27 *The Tin Pest Problem as a Test of Density Functionals Using High-Throughput Calculations*  
under review

**Authors:** M. J. Mehl, M. Ronquillo, D. Hicks, M. Esters, C. Oses, R. Friedrich, A. Smolyanyuk, E. Gossett, D. Finkenstadt & S. Curtarolo

**Abstract:** At ambient pressure tin transforms from its ground-state semi-metal  $\alpha$ -Sn (diamond structure) phase to the compact metallic  $\beta$ -Sn phase at 13°C (286K). There may be a further transition to the simple hexagonal  $\gamma$ -Sn above 450K. These relatively low transition temperatures are due to the small energy differences between the structures,  $\approx 20$  meV/atom between  $\alpha$ - and  $\beta$ -Sn. This makes tin an exceptionally sensitive test of the accuracy of density functionals and computational methods. Here we use the high-throughput Automatic-FLOW (AFLOW) method to study the energetics of tin in multiple structures using a variety of density functionals. We look at the successes and deficiencies of each functional. As no functional is completely satisfactory, we look Hubbard U corrections and show that the Coulomb interaction can be chosen to predict the correct phase transition temperature. We also discuss the necessity of testing high-throughput calculations for convergence for systems with small energy differences.

**arXiv:** [arxiv:2010.07168](https://arxiv.org/abs/2010.07168)

26 *Carbon Stoichiometry and Mechanical Properties of High Entropy Carbide*  
under review

**Authors:** M. D. Hossain<sup>†</sup>, T. Borman<sup>†</sup>, F. A. Kumar, X. Chen, A. Khosravani, S. R. Kalidindi, E. A. Paisley, M. Esters, C. Oses, C. Toher, S. Curtarolo, J. M. LeBeau, D. W. Brenner & J.-P. Maria

<sup>†</sup> contributed equally

**Abstract:** The search for new materials via compositional exploration has recently led to the discovery of entropy stabilized and high entropy ceramics. The chemical diversity in the cation sublattice of high entropy ceramics has led to many enhanced properties and applications such as reversible energy storage, low temperature water splitting, amorphous-like thermal transport in crystalline solids and enhanced mechanical properties. This work describes the synthesis and mechanical properties of high entropy (HfNbTaTiZr) $C_x$  thin films as a function of carbon content. The nature of the bonding and microstructure evolves as the material transforms from metallic to ceramic to nanocomposite with variations in the quantity and types of carbon, yielding large variations in the film hardness. Through multiple characterization techniques and first principles investigations, we separate the roles of microstructure and bonding characteristics in the mechanical property development of (HfNbTaTiZr) $C_x$  thin films. This study presents a strategy to establish the bonding, structure, and property relationships in chemically disordered high entropy ceramics, largely based on the relative populations of filled or empty antibonding states for which there are new abilities to do so in high configurational entropy systems that exhibit high solubility of diverse cations while retaining rocksalt structure.

25 *Fermi energy engineering of enhanced toughness in high entropy carbides*  
under review

**Authors:** T. J. Harrington<sup>†</sup>, C. Oses<sup>†</sup>, C. Toher, W. M. Mellor, K. Kaufmann, J. Gild, A. Wright, J. Luo, S. Curtarolo & K. S. Vecchio

<sup>†</sup> contributed equally

**Abstract:** Mechanical properties of a range of high entropy, rocksalt carbides are investigated via *ab-initio* modeling and experimental verification. Elastic constants, hardness, and fracture toughness depend on the electronic structure of the system which is parameterized through two descriptors: the valence electron concentration (VEC) and the integrated density of states from the pseudo-gap energy to the Fermi energy ( $iDOS(E_{pg}, E_F)$ ). Compositions incorporating more electrons (increasing VEC) shift  $E_F$  further above  $E_{pg}$ , increasing filling of the more deformable metal d-derived  $t_{2g}$  bonding orbitals. MoNbTaVWC5 — stabilizing as a single-phase rocksalt solid solution — has a VEC of 9.4, an  $iDOS(E_{pg}, E_F)$  of 7.66 states/cell, and a higher electron abundance than any of the rocksalt binary and ternary carbides. The material exhibits an experimental fracture toughness of  $2.91 \pm 0.27$  MPa·m<sup>1/2</sup> and a hardness of  $19.2 \pm 1.4$  GPa: a combination of high hardness and toughness rarely found in materials. Entropy, enabling high VEC in a cubic structure, highlights a new path for tailoring mechanical properties.

24 *On-the-fly Closed-loop Autonomous Materials Discovery via Bayesian Active Learning*  
Nat. Commun. **in press** (2020)

**Authors:** A. G. Kusne<sup>†</sup>, H. Yu<sup>†</sup>, C. Wu, H. Zhang, J. Hattrick-Simpers, B. DeCost, S. Sarker, C. Oses, C. Toher, S. Curtarolo, A. Davidov, R. Agarwal, L. Bendersky, M. Li, A. Mehta & I. Takeuchi

<sup>†</sup> contributed equally

**Abstract:** The search for advanced materials is hindered by the vast search space of compositions and the exceedingly complex synthesis-processes-structure-property landscape. We demonstrate autonomous research methodology (*i.e.* autonomous hypothesis definition and evaluation) that can place complex, advanced materials in reach, allowing scientists to fail smarter, learn faster, and spend less resources in their studies, while simultaneously improving trust in scientific results and machine learning tools. Additionally, robot science enables science- over-the-network, reducing the economic impact of scientists being separated from their labs. The real-time closed-loop, autonomous system for materials exploration and optimization (CAMEO) is used at the synchrotron beamline to accelerate the fundamentally interconnected tasks of rapid phase mapping and advanced-materials discovery, with each cycle taking seconds to minutes, resulting in the discovery of a novel nanocomposite phase-change memory material.



- 23 *Discovery of novel high-entropy ceramics via machine learning*  
NPJ Comput. Mater. **6**, 42 (2020)

**Authors:** K. Kaufmann, D. Maryanovsky, W. M. Mellor, C. Zhu, A. S. Rosengarten, T. J. Harrington, C. Oses, C. Toher, S. Curtarolo & K. S. Vecchio

**Abstract:** While high-entropy materials are attracting considerable interest due to a combination of useful properties and promising applications, predicting their formation remains a hindrance for rational discovery of new systems. Experimental approaches are based on physical intuition and/or expensive trial and error strategies. Most computational methods rely on the availability of sufficient experimental data and computational power. Machine learning (ML) applied to materials science can accelerate development and reduce costs. In this article, we propose a ML method leveraging thermodynamic and compositional attributes of a given material for predicting the synthesizability (*i.e.* entropy-forming-ability) of disordered metal carbides. The relative importance of the thermodynamic and compositional features for the predictions are then explored. The approach's suitability is demonstrated by comparing values calculated with density functional theory to ML predictions. Finally, the model is employed to predict the entropy-forming-ability of 70 new compositions; several predictions are validated by additional density functional theory calculations and experimental synthesis, corroborating the effectiveness in exploring vast compositional spaces in a high-throughput manner. Importantly, seven compositions are selected specifically because they contain all three of the Group VI elements (Cr, Mo, and W), which do not form room temperature stable rock-salt monocarbides. Incorporating the Group VI elements into the rock-salt structure provides further opportunity for tuning the electronic structure and potentially material performance.

DOI: [10.1038/s41524-020-0317-6](https://doi.org/10.1038/s41524-020-0317-6)

- 22 *High-entropy ceramics*  
Nat. Rev. Mater. **5**, 295–309 (2020)

**Authors:** C. Oses, C. Toher & S. Curtarolo

**Abstract:** Disordered multi-component systems, occupying the mostly uncharted centers of phase diagrams, were proposed in 2004 as innovative materials with promising applications. The idea was to maximize the configurational entropy to stabilize (near) equimolar mixtures and achieve more robust systems, which became known as high-entropy materials. Initial research focused mainly on metal alloys and nitride films. In 2015, entropy stabilization was demonstrated in a mixture of oxides. Other high-entropy disordered ceramics rapidly followed, stimulating the addition of more components to obtain materials expressing a blend of properties, often highly enhanced. The systems were soon proven to be useful in wide-ranging technologies, including thermal barrier coatings, thermoelectrics, catalysts, batteries, and wear-resistant and corrosion-resistant coatings. In this Review, we discuss the current state of the disordered ceramics field by examining the applications and the high-entropy features fueling them, covering both theoretical predictions and experimental results. The influence of entropy is unavoidable and can no longer be ignored. In the space of ceramics, it leads to new materials that, both as bulk and thin-films, will play important roles in technology in the decades to come.

DOI: [10.1038/s41578-019-0170-8](https://doi.org/10.1038/s41578-019-0170-8)

2019

- 21 *Metallic glasses for biodegradable implants*  
Acta Mater. **176**, 297–305 (2019)

**Authors:** D. C. Ford, D. Hicks, C. Oses, C. Toher & S. Curtarolo

**Abstract:** Metallic glasses are excellent candidates for biomedical implant applications due to their inherent strength and corrosion resistance. Use of metallic glasses in structural applications is limited, however, because bulk dimensions are challenging to achieve. Glass-forming ability (GFA) varies strongly with alloy composition and becomes more difficult to predict as the number of chemical species in a system increases. Here we present a theoretical model — implemented in the AFLOW framework — for predicting GFA based on the competition between crystalline phases, and apply it to biologically relevant binary and ternary systems. Elastic properties are estimated based on the rule of mixtures for alloy systems that are predicted to be bulk glass-formers. Focusing on Ca- and Mg-based systems for use in biodegradable orthopedic support applications, we suggest alloys in the AgCaMg and AgMgZn families for further study; and alloys based on the compositions:  $\text{Ag}_{0.33}\text{Mg}_{0.67}$ ,  $\text{Cu}_{0.5}\text{Mg}_{0.5}$ ,  $\text{Cu}_{0.37}\text{Mg}_{0.63}$  and  $\text{Cu}_{0.25}\text{Mg}_{0.5}\text{Zn}_{0.25}$ .

DOI: [10.1016/j.actamat.2019.07.008](https://doi.org/10.1016/j.actamat.2019.07.008)

- 20 *Predicting Superhard Materials via a Machine Learning Informed Evolutionary Structure Search*  
NPJ Comput. Mater. **5**, 89 (2019)

**Authors:** P. Avery, X. Wang, C. Oses, E. Gossett, D. M. Proserpio, C. Toher, S. Curtarolo & E. Zurek

**Abstract:** Good agreement was found between experimental Vickers hardnesses,  $H_V$ , of a wide range of materials and those calculated by three macroscopic hardness models that employ the shear and/or bulk moduli obtained from: (i) first principles via AFLOW-AEL (AFLOW Automatic Elastic Library), and (ii) a machine learning (ML) model trained on materials within the AFLOW repository. Because  $H_V$ ML values can be quickly estimated, they can be used in conjunction with an evolutionary search to predict stable, superhard materials. This methodology is implemented in the XTALOPT evolutionary algorithm. Each crystal is minimized to the nearest local minimum, and its Vickers hardness is computed via a linear relationship with the shear modulus discovered by Teter. Both the energy/enthalpy and  $H_{V,Teter}^{ML}$  are employed to determine a structure's fitness. This implementation is applied towards the carbon system, and 43 new superhard phases are found. A topological analysis reveals that phases estimated to be slightly harder than diamond contain a substantial fraction of diamond and/or lonsdaleite.

DOI: [10.1038/s41524-019-0226-8](https://doi.org/10.1038/s41524-019-0226-8)

- 19 *Unavoidable disorder and entropy in multi-component systems*  
NPJ Comput. Mater. **5**, 69 (2019)

**Authors:** C. Toher, C. Oses, D. Hicks & S. Curtarolo

**Abstract:** The need for improved functionalities is driving the search for more complicated multi-component materials. The competition between enthalpy and entropy is unveiled by statistical analysis of big-data repositories. A threshold in the number of species is found. Beyond that, enthalpy can be neglected, and disorder — complete or partial — is unavoidable.

**DOI:** [10.1038/s41524-019-0206-z](https://doi.org/10.1038/s41524-019-0206-z)

- 18 *Coordination corrected *ab initio* formation enthalpies*  
NPJ Comput. Mater. **5**, 59 (2019)

**Authors:** R. Friedrich, D. Usanmaz, C. Oses, A. R. Supka, M. Fornari, M. Buongiorno Nardelli, C. Toher & S. Curtarolo

**Abstract:** The correct calculation of formation enthalpy is one of the enablers of *ab-initio* computational materials design. For several classes of systems (*e.g.* oxides) standard density functional theory produces incorrect values. Here we propose the “coordinationcorrected-enthalpies” method (CCE), based on the number of nearest neighbor cation-anion bonds, and also capable of correcting relative stability of polymorphs. The approach uses calculations employing the PBE, LDA and SCAN exchange correlation functionals, in conjunction with a quasiharmonic Debye model to treat zero-point vibrational and thermal effects. The benchmark, performed on binary and ternary oxides, shows very accurate room temperature results for all functionals, with the smallest mean absolute error of 27 meV/atom obtained with SCAN. The zero-point vibrational and thermal contributions to the formation enthalpies are small and with different signs — largely cancelling each other.

**DOI:** [10.1038/s41524-019-0192-1](https://doi.org/10.1038/s41524-019-0192-1)

- 17 *AFLOW-QHA3P: Robust and automated method to compute thermodynamic properties of solids*  
Phys. Rev. Mater. **3**, 073801 (2019)

**Authors:** P. Nath, D. Usanmaz, D. Hicks, C. Oses, M. Fornari, M. Buongiorno Nardelli, C. Toher & S. Curtarolo

**Abstract:** Accelerating the calculations of finite-temperature thermodynamic properties is a major challenge for rational materials design. Reliable methods can be quite expensive, limiting their applicability in autonomous high-throughput workflows. Here, the three-phonon quasi-harmonic approximation (QHA) method is introduced, requiring only three phonon calculations to obtain a thorough characterization of the material. Leveraging a Taylor expansion of the phonon frequencies around the equilibrium volume, the method efficiently resolves the volumetric thermal expansion coefficient, specific heat at constant pressure, the enthalpy, and bulk modulus. Results from the standard QHA and experiments corroborate the procedure, and additional comparisons are made with the recently developed self-consistent QHA. The three approaches — three-phonon, standard, and self-consistent QHAs — are all included within the open-source framework AFLOW, allowing automated determination of properties with various implementations within the same framework.

**DOI:** [10.1103/PhysRevMaterials.3.073801](https://doi.org/10.1103/PhysRevMaterials.3.073801)

2018

- 16 *AFLOW-CHULL: Cloud-oriented platform for autonomous phase stability analysis*  
J. Chem. Inf. Model. **58**(12), 2477–2490 (2018)

**Authors:** C. Oses, E. Gossett, D. Hicks, F. Rose, M. J. Mehl, E. Perim, I. Takeuchi, S. Sanvito, M. Scheffler, Y. Lederer, O. Levy, C. Toher & S. Curtarolo

**Abstract:** *A priori* prediction of phase stability of materials is a challenging practice, requiring knowledge of all energetically-competing structures at formation conditions. Large materials repositories — housing properties of both experimental and hypothetical compounds — offer a path to prediction through the construction of informatics-based, *ab-initio* phase diagrams. However, limited access to relevant data and software infrastructure has rendered thermodynamic characterizations largely peripheral, despite their continued success in dictating synthesizability. Herein, a new module is presented for autonomous thermodynamic stability analysis implemented within the open-source, *ab-initio* framework AFLOW. Powered by the AFLUX Search-API, AFLOW-CHULL leverages data of more than 1.8 million compounds currently characterized in the AFLOW.org repository and can be employed locally from any UNIX-like computer. The module integrates a range of functionality: the identification of stable phases and equivalent structures, phase coexistence, measures for robust stability, and determination of decomposition reactions. As a proof-of-concept, thorough thermodynamic characterizations have been performed for more than 1,300 binary and ternary systems, enabling the identification of several candidate phases for synthesis based on their relative stability criterion — including 18 promising C15<sub>b</sub>-type structures and two half-Heuslers. In addition to a full report included herein, an interactive, online web application has been developed showcasing the results of the analysis, and is located at [aflow.org/aflow-chull](http://aflow.org/aflow-chull).

**DOI:** [10.1021/acs.jcim.8b00393](https://doi.org/10.1021/acs.jcim.8b00393)



- 15 *Data-driven design of inorganic materials with the Automatic Flow Framework for Materials Discovery*  
MRS Bull. **43**(9), 670–675 (2018)

**Authors:** C. Oses, C. Toher & S. Curtarolo

**Abstract:** The expansion of programmatically-accessible materials data has cultivated opportunities for data-driven approaches. Workflows such as the Automatic Flow Framework for Materials Discovery not only manage the generation, storage, and dissemination of materials data, but also leverage the information for thermodynamic formability modeling, such as the prediction of phase diagrams and properties of disordered materials. In combination with standardized parameter sets, the wealth of data is ideal for training machine learning algorithms, which have already been employed for property prediction, descriptor development, design rule discovery, and the identification of candidate functional materials. These methods promise to revolutionize the path to synthesis and, ultimately, transform the practice of traditional materials discovery to one of rational and autonomous materials design.

**DOI:** [10.1557/mrs.2018.207](https://doi.org/10.1557/mrs.2018.207)

- 14 *Novel high-entropy high-hardness metal carbides discovered by entropy descriptors*  
Nat. Commun. **9**, 4980 (2018)

**Authors:** P. Sarker<sup>†</sup>, T. J. Harrington<sup>†</sup>, C. Toher, C. Oses, M. Samiee, J.-P. Maria, D. W. Brenner, K. S. Vecchio & S. Curtarolo

<sup>†</sup> contributed equally

**Abstract:** High-entropy materials have attracted considerable interest due to the combination of useful properties and promising applications. Predicting their formation remains the major hindrance to the discovery of new systems. Here we propose a descriptor — entropy forming ability — for addressing synthesizability from first principles. The formalism, based on the energy distribution spectrum of randomized calculations, captures the accessibility of equally-sampled states near the ground state and quantifies configurational disorder capable of stabilizing high-entropy homogeneous phases. The methodology is applied to disordered refractory 5-metal carbides — promising candidates for high-hardness applications. The descriptor correctly predicts the ease with which compositions can be experimentally synthesized as rock-salt high-entropy homogeneous phases, validating the ansatz, and in some cases, going beyond intuition. Several of these materials exhibit hardness up to 50% higher than rule of mixtures estimations. The entropy descriptor method has the potential to accelerate the search for high-entropy systems by rationally combining first principles with experimental synthesis and characterization.

**DOI:** [10.1038/s41467-018-07160-7](https://doi.org/10.1038/s41467-018-07160-7)

- 13 *Machine learning modeling of superconducting critical temperature*  
NPJ Comput. Mater. **4**, 29 (2018)

**Authors:** V. Stanev, C. Oses, A. G. Kusne, E. Rodriguez, J. Paglione, S. Curtarolo & I. Takeuchi

**Abstract:** Superconductivity has been the focus of enormous research effort since its discovery more than a century ago. Yet, some features of this unique phenomenon remain poorly understood; prime among these is the connection between superconductivity and chemical/structural properties of materials. To bridge the gap, several machine learning methods are developed herein to model the critical temperatures ( $T_c$ ) of the 12,000+ known superconductors available via the SuperCon database. Materials are first divided into two classes based on their  $T_c$ 's, above and below 10 K, and a classification model predicting this label is trained. The model uses coarse-grained features based only on the chemical compositions. It shows strong predictive power, with out-of-sample accuracy of about 92%. Separate regression models are developed to predict the values of  $T_c$  for cuprate, iron-based, and “low- $T_c$ ” compounds. These models also demonstrate good performance, with learned predictors offering important insights into the mechanisms behind superconductivity in different families of materials. To improve the accuracy and interpretability of these models, new features are incorporated using materials data from the AFLOW Online Repositories. Finally, the classification and regression models are combined into a single integrated pipeline and employed to search the entire Inorganic Crystallographic Structure Database (ICSD) for potential new superconductors. We identify about 30 non-cuprate and non-iron-based oxides as candidate materials.

**DOI:** [10.1038/s41524-018-0085-8](https://doi.org/10.1038/s41524-018-0085-8)

- 12 *AFLOW-ML: A RESTful API for machine-learning prediction of materials properties*  
Comput. Mater. Sci. **152**, 134–145 (2018)

**Authors:** E. Gossett, C. Toher, C. Oses, O. Isayev, F. Legrain, F. Rose, E. Zurek, J. Carrete, N. Mingo, A. Tropsha & S. Curtarolo

**Abstract:** Machine learning approaches, enabled by the emergence of comprehensive databases of materials properties, are becoming a fruitful direction for materials analysis. As a result, a plethora of models have been constructed and trained on existing data to predict properties of new systems. These powerful methods allow researchers to target studies only at interesting materials — neglecting the non-synthesizable systems and those without the desired properties — thus reducing the amount of resources spent on expensive computations and/or time-consuming experimental synthesis. However, using these predictive models is not always straightforward. Often, they require a panoply of technical expertise, creating barriers for general users. AFLOW-ML (AFLOW Machine Learning) overcomes the problem by streamlining the use of the machine learning methods developed within the AFLOW consortium. The framework provides an open RESTful API to directly access the continuously updated algorithms, which can be transparently integrated into any workflow to retrieve predictions of electronic, thermal and mechanical properties. These types of interconnected cloud-based applications are envisioned to be capable of further accelerating the adoption of machine learning methods into materials development.

• This paper was selected for [Editor's Choice](#).

**DOI:** [10.1016/j.commatsci.2018.03.075](https://doi.org/10.1016/j.commatsci.2018.03.075)

- 11 *AFLOW-SYM: platform for the complete, automatic and self-consistent symmetry analysis of crystals*  
Acta Cryst. A **74**, 184–203 (2018)  
**Authors:** D. Hicks, C. Oses, E. Gossett, G. Gomez, R. H. Taylor, C. Toher, M. J. Mehl, O. Levy & S. Curtarolo  
**Abstract:** Determination of the symmetry profile of structures is a persistent challenge in materials science. Results often vary amongst standard packages, hindering autonomous materials development by requiring continuous user attention and educated guesses. This article presents a robust procedure for evaluating the complete suite of symmetry properties, featuring various representations for the point, factor and space groups, site symmetries and Wyckoff positions. The protocol determines a system-specific mapping tolerance that yields symmetry operations entirely commensurate with fundamental crystallographic principles. The self-consistent tolerance characterizes the effective spatial resolution of the reported atomic positions. The approach is compared with the most used programs and is successfully validated against the space-group information provided for over 54,000 entries in the Inorganic Crystal Structure Database (ICSD). Subsequently, a complete symmetry analysis is applied to all 1.7+ million entries of the AFLOW data repository. The AFLOW-SYM package has been implemented in, and made available for, public use through the automated *ab initio* framework AFLOW.  
**DOI:** [10.1107/S2053273318003066](https://doi.org/10.1107/S2053273318003066)
- 2017
- 10 *The structure and composition statistics of 6A binary and ternary structures*  
Inorg. Chem. **57**(2), 653–667 (2017)  
**Authors:** A. Hever, C. Oses, S. Curtarolo, O. Levy & A. Natan  
**Abstract:** The fundamental principles underlying the arrangement of the elements into solid compounds with an enormous variety of crystal structures are still largely unknown. This study presents a general overview of the structure types appearing in an important subset of the solid compounds, *i.e.*, binary and ternary compounds of the 6A column oxides, sulfides and selenides. It contains an analysis of these compounds, including the prevalence of various structure types, their symmetry properties, compositions, stoichiometries and unit cell sizes. It is found that these compound families include preferred stoichiometries and structure types, some of which have highly specific atomic compositions that may reflect both their specific chemistry and research bias in the available empirical data.  
**DOI:** [10.1021/acs.inorgchem.7b02462](https://doi.org/10.1021/acs.inorgchem.7b02462)
- 9 *AFLUX: The LUX materials search API for the AFLOW data repositories*  
Comput. Mater. Sci. **137**, 362–370 (2017)  
**Authors:** F. Rose, C. Toher, E. Gossett, C. Oses, M. Buongiorno Nardelli, M. Fornari & S. Curtarolo  
**Abstract:** Automated computational materials science frameworks rapidly generate large quantities of materials data for accelerated materials design. In order to take advantage of these large databases, users should have the ability to efficiently search and extract the desired data. Therefore, we have extended the data oriented AFLOW-repository Application-Program-Interface (API) (Comput. Mater. Sci. **93**, 178 (2014)) to enable programmatic access to search queries. A Uniform Resource Identifier (URI)-based search API is proposed for the construction of complex queries for remote creation and retrieval of customized data sets. It is expected that the new language AFLUX, from Automatic Flow of LUX (light), will enable remote search operations on the AFLOW set of computational materials science data repositories. In addition, AFLUX facilitates the verification and validation of the data in the AFLOW repositories.  
• This paper was selected for [Editor's Choice](#).  
**DOI:** [10.1016/j.commatsci.2017.04.036](https://doi.org/10.1016/j.commatsci.2017.04.036)
- 8 *Universal Fragment Descriptors for Predicting Properties of Inorganic Crystals*  
Nat. Commun. **8**, 15679 (2017)  
**Authors:** O. Isayev<sup>†</sup>, C. Oses<sup>†</sup>, C. Toher, E. Gossett, S. Curtarolo & A. Tropsha  
<sup>†</sup> contributed equally  
**Abstract:** Historically, materials discovery is driven by a laborious trial-and-error process. The growth of materials databases and emerging informatics approaches finally offer the opportunity to transform this practice into data- and knowledge-driven rational design-accelerating discovery of novel materials exhibiting desired properties. By using data from the AFLOW repository for high-throughput ab-initio calculations, we have generated Quantitative Materials Structure-Property Relationship (QMSPR) models to predict three critical material properties, namely the metal / insulator classification, Fermi energy, and band gap energy. The prediction accuracy obtained with these QMSPR models approaches training data for virtually any stoichiometric inorganic crystalline material. We attribute the success and universality of these models to the construction of new material descriptors-referred to as the universal property-labeled material fragments (PLMF). This representation affords straightforward model interpretation in terms of simple heuristic design rules that could guide rational materials design. This proof-of-concept study demonstrates the power of materials informatics to dramatically accelerate the search for new materials.  
**DOI:** [10.1038/ncomms15679](https://doi.org/10.1038/ncomms15679)

- 7 *Combining the AFLOW GIBBS and elastic libraries to efficiently and robustly screening thermomechanical properties of solids*  
Phys. Rev. Mater. **1**, 015401 (2017)

**Authors:** C. Toher, C. Oses, J. J. Plata, D. Hicks, F. Rose, O. Levy, M. de Jong, M. Asta, M. Fornari, M. Buongiorno Nardelli & S. Curtarolo

**Abstract:** Thorough characterization of the thermomechanical properties of materials requires difficult and time-consuming experiments. This severely limits the availability of data and is one of the main obstacles for the development of effective accelerated materials design strategies. The rapid screening of new potential systems requires highly integrated, sophisticated, and robust computational approaches. We tackled the challenge by developing an automated, integrated workflow with robust error-correction within the AFLOW framework which combines the newly developed “Automatic Elasticity Library” with the previously implemented GIBBS method. The first extracts the mechanical properties from automatic self-consistent stress-strain calculations, while the latter employs those mechanical properties to evaluate the thermodynamics within the Debye model. The new thermoelastic library is benchmarked against a set of 74 experimentally characterized systems to pinpoint a robust computational methodology for the evaluation of bulk and shear moduli, Poisson ratios, Debye temperatures, Grüneisen parameters, and thermal conductivities of a wide variety of materials. The effect of different choices of equations of state and exchange-correlation functionals is examined and the optimum combination of properties for the Leibfried-Schlömann prediction of thermal conductivity is identified, leading to improved agreement with experimental results than the GIBBS-only approach. The framework has been applied to the AFLOW.org data repositories to compute the thermoelastic properties of over 3500 unique materials. The results are now available online by using an expanded version of the REST-API described in the Appendix.

**DOI:** [10.1103/PhysRevMaterials.1.015401](https://doi.org/10.1103/PhysRevMaterials.1.015401)

- 6 *A Computational High-Throughput Search for New Ternary Superalloys*  
Acta Mater. **122**, 438–447 (2017)

**Authors:** C. Nyshadham, C. Oses, J. E. Hansen, I. Takeuchi, S. Curtarolo & G. L. Hart

**Abstract:** In 2006, a novel cobalt-based superalloy was discovered with mechanical properties better than some conventional nickel-based superalloys. As with conventional superalloys, its high performance arises from the precipitate-hardening effect of a coherent L1<sub>2</sub> phase, which is in two-phase equilibrium with the fcc matrix. Inspired by this unexpected discovery of an L1<sub>2</sub> ternary phase, we performed a first-principles search through 2224 ternary metallic systems for analogous precipitate-hardening phases of the form X<sub>3</sub>[A<sub>0.5</sub>B<sub>0.5</sub>], where X = Ni, Co, or Fe, and [A, B] = Li, Be, Mg, Al, Si, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Sr, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn, Sb, Hf, Ta, W, Re, Os, Ir, Pt, Au, Hg, or Tl. We found 102 systems that have a smaller decomposition energy and a lower formation enthalpy than the Co<sub>3</sub>(Al, W) superalloy. They have a stable two-phase equilibrium with the host matrix within the concentration range  $0 < x < 1$  (X<sub>3</sub>[A<sub>x</sub>B<sub>1-x</sub>]) and have a relative lattice mismatch with the host matrix of less than or equal to 5%. These new candidates, narrowed from 2224 systems, suggest possible experimental exploration for identifying new superalloys. Of these 102 systems, 37 are new; they have no reported phase diagrams in standard databases. Based on cost, experimental difficulty, and toxicity, we limit these 37 to a shorter list of six promising candidates of immediate interest. Our calculations are consistent with current experimental literature where data exists.

**DOI:** [10.1016/j.actamat.2016.09.017](https://doi.org/10.1016/j.actamat.2016.09.017)

- 5 *Accelerated Discovery of New Magnets in the Heusler Alloy Family*  
Sci. Adv. **3**(4), e1602241 (2017)

**Authors:** S. Sanvito, C. Oses, J. Xue, A. Tiwari, M. Žic, T. Archer, P. Tozman, M. Venkatesan, J. D. Coey & S. Curtarolo

**Abstract:** Magnetic materials underpin modern technologies, ranging from data storage to energy conversion to contactless sensing. However, the development of a new high-performance magnet is a long and often unpredictable process, and only about two dozen feature in mainstream applications. We describe a systematic pathway to the design of novel magnetic materials, which demonstrates a high throughput and discovery speed. On the basis of an extensive electronic structure library of Heusler alloys containing 236,115 prototypical compounds, we filtered those alloys displaying magnetic order and established whether they can be fabricated at thermodynamical equilibrium. Specifically, we carried out a full stability analysis of intermetallic Heusler alloys made only of transition metals. Among the possible 36,540 prototypes, 248 were thermodynamically stable but only 20 were magnetic. The magnetic ordering temperature, T<sub>C</sub>, was estimated by a regression calibrated on the experimental T<sub>C</sub> of about 60 known compounds. As a final validation, we attempted the synthesis of a few of the predicted compounds and produced two new magnets: Co<sub>2</sub>MnTi, which displays a remarkably high T<sub>C</sub> in perfect agreement with the predictions, and Mn<sub>2</sub>PtPd, which is an antiferromagnet. Our work paves the way for large-scale design of novel magnetic materials at potentially high speed.

**DOI:** [10.1126/sciadv.1602241](https://doi.org/10.1126/sciadv.1602241)

2016

- 4 *High-Throughput Computation of Thermal Conductivity of High-Temperature Solid Phases: The Case of Oxide and Fluoride Perovskites*  
Phys. Rev. X **6**(4), 041061 (2016)

**Authors:** A. van Roekeghem, J. Carrete, C. Oses, S. Curtarolo & N. Mingo

**Abstract:** Using finite-temperature phonon calculations and machine-learning methods, we assess the mechanical stability of about 400 semiconducting oxides and fluorides with cubic perovskite structures at 0, 300, and 1000 K. We find 92 mechanically stable compounds at high temperatures — including 36 not mentioned in the literature so far — for which we calculate the thermal conductivity. We show that the thermal conductivity is generally smaller in fluorides than in oxides, largely due to a lower ionic charge, and describe simple structural descriptors that are correlated with its magnitude. Furthermore, we show that the thermal conductivities of most cubic perovskites decrease more slowly than the usual  $T^{-1}$  behavior. Within this set, we also screen for materials exhibiting negative thermal expansion. Finally, we describe a strategy to accelerate the discovery of mechanically stable compounds at high temperatures.

**DOI:** [10.1103/PhysRevX.6.041061](https://doi.org/10.1103/PhysRevX.6.041061)

- 3 *Modeling Off-Stoichiometry Materials with a High-Throughput Ab-Initio Approach*  
Chem. Mater. **28**(18), 6484–6492 (2016)

**Authors:** K. Yang, C. Oses & S. Curtarolo

**Abstract:** Predicting material properties of off-stoichiometry systems remains a long-standing and formidable challenge in rational materials design. A proper analysis of such systems by means of a supercell approach requires the exhaustive consideration of all possible superstructures, which can be a time-consuming process. On the contrary, the use of quasirandom approximants, although very computationally effective, implicitly bias the analysis toward disordered states with the lowest site correlations. Here, we propose a novel framework designed specifically to investigate stoichiometrically driven trends of disordered systems (*i.e.*, having partial occupation and/or disorder in the atomic sites). At the heart of the approach is the identification and analysis of unique supercells of a virtually equivalent stoichiometry to the disordered material. We employ Boltzmann statistics to resolve system-wide properties at a high-throughput (HT) level. To maximize efficiency and accessibility, we integrated the method within the automatic HT computational framework AFLOW. As proof of concept, we apply our approach to three systems of interest, a zinc chalcogenide ( $\text{ZnS}_{1-x}\text{Se}_x$ ), a wide-gap oxide semiconductor ( $\text{Mg}_x\text{Zn}_{1-x}\text{O}$ ), and an iron alloy ( $\text{Fe}_{1-x}\text{Cu}_x$ ), at various stoichiometries. These systems exhibit properties that are highly tunable as a function of composition, characterized by optical bowing and linear ferromagnetic behavior. Not only are these qualities successfully predicted, but additional insight into underlying physical mechanisms is revealed.

**DOI:** [10.1021/acs.chemmater.6b01449](https://doi.org/10.1021/acs.chemmater.6b01449)

2015

- 2 *The AFLOW Standard for High-Throughput Materials Science Calculations*  
Comput. Mater. Sci. **108A**, 233–238 (2015)

**Authors:** C. E. Calderon, J. J. Plata, C. Toher, C. Oses, O. Levy, M. Fornari, A. Natan, M. J. Mehl, G. L. Hart, M. Buongiorno Nardelli & S. Curtarolo

**Abstract:** The Automatic-Flow (AFLOW) standard for the high-throughput construction of materials science electronic structure databases is described. Electronic structure calculations of solid state materials depend on a large number of parameters which must be understood by researchers, and must be reported by originators to ensure reproducibility and enable collaborative database expansion. We therefore describe standard parameter values for k-point grid density, basis set plane wave kinetic energy cut-off, exchange-correlation functionals, pseudopotentials, DFT+U parameters, and convergence criteria used in AFLOW calculations.

- This paper was selected for [Editor's Choice](#).

**DOI:** [10.1016/j.commatsci.2015.07.019](https://doi.org/10.1016/j.commatsci.2015.07.019)

- 1 *Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints*  
Chem. Mater. **27**(3), 735–743 (2015)

**Authors:** O. Isayev, D. Fourches, E. N. Muratov, C. Oses, K. M. Rasch, A. Tropsha & S. Curtarolo

**Abstract:** As the proliferation of high-throughput approaches in materials science is increasing the wealth of data in the field, the gap between accumulated-information and derived-knowledge widens. We address the issue of scientific discovery in materials databases by introducing novel analytical approaches based on structural and electronic materials fingerprints. The framework is employed to (i) query large databases of materials using similarity concepts, (ii) map the connectivity of materials space (*i.e.*, as a materials cartograms) for rapidly identifying regions with unique organizations / properties, and (iii) develop predictive Quantitative Materials Structure-Property Relationship models for guiding materials design. In this study, we test these fingerprints by seeking target material properties. As a quantitative example, we model the critical temperatures of known superconductors. Our novel materials fingerprinting and materials cartography approaches contribute to the emerging field of materials informatics by enabling effective computational tools to analyze, visualize, model, and design new materials.

- This paper was selected for [Editor's Choice](#).

**DOI:** [10.1021/cm503507h](https://doi.org/10.1021/cm503507h)