COREY OSES

Materials Science, Duke University

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

Proficient Coder — Present — `C++`, `Python`, LaTeX, `MATLAB` & `R`

Postdoctoral Fellow — 2018–present — Duke University
Supervisor: Stefano Curtarolo

Internship — 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).
Supervisors: Richard E. Gillilan & Ernest Fontes

Internship — 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.
Supervisors: Rong Huang & Ernest Fontes

Office Assistant — Summer 2011 — ILR Budget Office, Cornell University
Supervisor: Renee Monroe Cook

Externship — March 2010 — Supreme Court of New York
Supervisors: Ariel E. Belen & Allen Hurkin-Torres

Math Tutor — Fall 2008 — Graduate Record Exam (GRE)

Office Assistant — Summer 2008 — SOS Security, LLC in Parsippany, NJ
Supervisor: James Flanagan

EDUCATION

Ph.D. — 2013–2018 — Duke University
GPA: 3.8/4.0 · **Department**: Mechanical Engineering and Materials Science
Thesis: *Machine learning, phase stability, and disorder with the Automatic Flow Framework for Materials Discovery*
ProQuest: search.proquest.com/docview/2172402640?pq-origsite=gscholar
Advisor: Stefano Curtarolo

B.Sc. — 2009–2013 — Cornell University
GPA: 3.3/4.0 · **Department**: Applied and Engineering Physics
Thesis: *Plume Propagation Simulation for Pulsed Laser Deposition*
Advisor: Joel Brock

High School Diploma — 2005–2009 — Bloomfield High School
GPA: 3.9/4.0 · *Graduated fifth in class of 428*

PRESS AND NEWS RELEASES

Duke University Pratt School of Engineering — November 2018 — *"Disordered Materials Could Be Hardest, Most Heat-Tolerant Ever"*

- This press release is featured on AAAS EurekAlert!, Phys.org, ScienceDaily, Science Bulletin, Naaju, NewsBeezer, RemoNews, Tech2, and LongRoom News.

pratt.duke.edu/about/news/chaotic-carbides

Diversity in Action — September 2018 — *"Options in Education: Building Bridges — Pratt School of Engineering mentors underrepresented students"*

bluetoad.com/publication/?i=521423&ver=html5&p=70#&

MRS Bulletin — August 2017 — *"Universal fragment descriptor predicts materials properties"*

cambridge.org/core/journals/mrs-bulletin/news/universal-fragment-descriptor-predicts-materials-properties

UNC Eshelman School of Pharmacy — June 2017 — *"Breakthrough Tool Predicts Properties of Theoretical Materials, Finds New Uses for Current Ones"*

- This press release is featured on AAAS EurekAlert!, Phys.org, and ScienceDaily.

pharmacy.unc.edu/news/2017/06/06/breakthrough-tool-predicts-properties-theoretical-materials-finds-new-uses-current-ones/

Duke University Pratt School of Engineering — April 2017 — *"Computers Create Recipe for Two New Magnetic Materials"*

- This press release is featured on Phys.org, Slashdot, Hacker News, Reddit, Engadget, Engineering.com, Science Alert, Azo Materials, Next Big Future, Futurism, New Atlas, and International Business Times.

pratt.duke.edu/about/news/predicting-magnets

MRS Bulletin — April 2015 — *"Materials fingerprints identified for informatics"*

doi.org/10.1557/mrs.2015.76

Computational Chemistry Highlights — January 2015 — *"Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints"*

- "This paper is a *tour de force* for computational materials science" — Prof. Alán Aspuru-Guzik, Harvard University.

compchemhighlights.org/2015/01/materials-cartography-representing-and.html

Duke University Research — January 2015 — *"Molecular Tornado"*

research.duke.edu/molecular-tornado

Duke University Graduate School — October 2014 — *"Competing for NSF Fellowships: Advice from a Current Fellow"*

gradschool.duke.edu/professional-development/blog/competing-nsf-fellowships-advice-current-fellow

Duke University Pratt School of Engineering — June 2014 — *"Pratt Profiles: Corey Oses"*

pratt.duke.edu/graduate/diversity/pratt-profiles-corey-oses

Duke University MEM Program — November 2013 — *"Society of Hispanic Professional Engineers"*

memp.pratt.duke.edu/news/society-hispanic-professional-engineers

New York Kiwanis — February 2013 — *"New York Kiwanis Mid-Winter Conference 2013"*

kiwanis-ny.org/1213/midyear.htm

ERN Conference 2013 — February 2013 — *"2013 Oral and Poster Presentation Award Winners"*

new.emerging-researchers.org/2013-oral-and-poster-presentation-winners

New York Kiwanis — June 2012 — *"K-Kids Show Talent for Fundraising"*

patch.com/new-york/eastmeadow/k-kids-show-talent-for-fundraising

New York Kiwanis — March 2012 — *"Past Circle K Governors Help Celebrate 50th Convention"*

Elected Governor of New York Circle K.
kiwanis-ny.org/news/view_news.php?nid=618

HONORS AND AWARDS

Award — November 09, 2018 — Presentation Finalist at the Engineering Science Symposium, SHPE National Conference

Publication Award	2018	Editor's Choice, Publication in Comput. Mater. Sci., Elsevier
Award	November 03, 2017	Presentation Winner at the Engineering Science Symposium, SHPE National Conference
Publication Award	2017	Editor's Choice, Publication in Comput. Mater. Sci., Elsevier
Award	November 04, 2016	Presentation Finalist at the Engineering Science Symposium, SHPE National Conference
Award	August 14, 2015	Best Teaching Assistant Award (ME 221), Duke University Department of Mechanical Engineering and Materials Science
Publication Award	2015	Editor's Choice, Publication in Comput. Mater. Sci., Elsevier
Publication Award	2015	Editor's Choice, Publication in Chem. Mater., American Chemical Society
Fellowship	2013–2016	Graduate Research Fellowship, National Science Foundation
Fellowship	2013–2015	Associate Fellow, National GEM Consortium
Award	November 01, 2013	Technical Poster and Paper Finalist at the Engineering Science Symposium, SHPE National Conference
Award	August 22, 2013	Best Presentation Award at the MEMS Departmental Retreat, Duke University Department of Mechanical Engineering and Materials Science
City Citation	March 21, 2013	New York City Citation as Circle K Governor, Council Member Fernando Cabrera
Award	March 02, 2013	First Place in Nanoscience and Physics Research Presentation, NSF / AAAS / EHR Emerging Researchers National Conference
Award	October 08, 2011	College Bowl Winner, Hispanic Engineer National Achievement Awards Conference (HENAAC)
	Northrop Grumman One Team	
Scholarship	2011–2013	Shell Incentive Fund Scholarship
Honor	2010–2013	Louis Stokes Alliance for Minority Participation (LSAMP) Scholar
Scholarship	2010 & 2011	Xerox Corporation Scholarship
Scholarship	2010 & 2011	Intel Academic Award
Scholarship	2010–2013	GE Foundation / LULAC Scholarship
Grant	June 18, 2010	Cornell University Unmanned Air Systems Team awarded $1,000 grant, AUVSI Student Unmanned Aerial Systems Competition
Scholarship	2009–2013	Meinig Family Cornell National Scholars
	Awarded by Peter Meinig (Past Chairman of the Board of Trustees at Cornell University)	
Scholarship	2009	*Men of Principle* Award, Beta Theta Pi
	Beta Delta Chapter	
Scholarship	2009	Gold Medallion Winner in Engineering and Mathematics, Hispanic Heritage Youth Awards
Scholarship	2009	New Jersey Principals and Supervisors Association Scholarship
Scholarship	2009	Edward J. Bloustein Distinguished Scholar
Scholarship	2009	Investors Savings Bank Scholarship
Scholarship	2009	Bloomfield Education Association Scholarship
Scholarship	2009	Special Recognition Award, Bloomfield Kiwanis
Scholarship	2009	The Harold Brotherhood Award

Scholarship	2009	Jean Doswell Oakes Scholarship, Oakeside Cultural Center
Scholarship	2009	Superintendent's Bengal Pride Award for Excellence in Academics and Citizenship
Award	2009	Outstanding Student Citizen for Youth Week, Bloomfield High School
Award	2009	First Place Impromptu Essay, New Jersey Key Club Convention
Scholarship	2009	Good Citizen Award, The Daughters of the American Revolution
Honor	2008–2009	National Honor Society
Honor	2008–2009	Scholar Athlete, Bloomfield High School
Honor	2006–2009	Academic Excellence, Bloomfield High School
Honor	2008	National Ventures Scholar Program
Award	2008	Yale Book Club Award, Yale Club of Montclair, New Jersey

Journal Publications

2020

Under Review 24 *Fermi energy engineering of enhanced toughness in high entropy carbides*

Authors: Tyler J. Harrington[†], Corey Oses[†], Cormac Toher, William M. Mellor, Kevin Kaufmann, Joshua Gild, Andrew Wright, Jian Luo, Stefano Curtarolo & Kenneth S. Vecchio
[†] 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 ± 0.27 MPa·m$^{1/2}$ and a hardness of 19.2 ± 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.

Under Review 23 *Discovery of novel high-entropy ceramics via machine learning*

Authors: Kevin Kaufmann, Daniel Maryanovsky, William M. Mellor, Chaoyi Zhu, Alexander S. Rosengarten, Tyler J. Harrington, Corey Oses, Cormac Toher, Stefano Curtarolo & Kenneth 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.

Nature Reviews Materials

22 *High-entropy ceramics*
Nat. Rev. Mater. (2020)

Authors: Corey Oses, Cormac Toher & Stefano 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

2019

Acta Materialia

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

Authors: Denise C. Ford, David Hicks, Corey Oses, Cormac Toher & Stefano 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: $Ag_{0.33}Mg_{0.67}$, $Cu_{0.5}Mg_{0.5}$, $Cu_{0.37}Mg_{0.63}$ and $Cu_{0.25}Mg_{0.5}Zn_{0.25}$.
DOI: 10.1016/j.actamat.2019.07.008

NPJ Computational Materials

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

Authors: Patrick Avery, Xiaoyu Wang, Corey Oses, Eric Gossett, Davide M. Proserpio, Cormac Toher, Stefano Curtarolo & Eva 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_VML 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 $H^{ML}_{V,Teter}$ 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

NPJ Computational Materials

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

Authors: Cormac Toher, Corey Oses, David Hicks & Stefano 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

NPJ Computational Materials

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

Authors: Rico Friedrich, Demet Usanmaz, Corey Oses, Andrew R. Supka, Marco Fornari, Marco Buongiorno Nardelli, Cormac Toher & Stefano 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

Physical Review Materials

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

Authors: Pinku Nath, Demet Usanmaz, David Hicks, Corey Oses, Marco Fornari, Marco Buongiorno Nardelli, Cormac Toher & Stefano 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

2018

Journal of Chemical Information and Modeling

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

Authors: Corey Oses, Eric Gossett, David Hicks, Frisco Rose, Michael J. Mehl, Eric Perim, Ichiro Takeuchi, Stefano Sanvito, Matthias Scheffler, Yoav Lederer, Ohad Levy, Cormac Toher & Stefano 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 $C15_b$-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.
DOI: 10.1021/acs.jcim.8b00393

MRS Bulletin

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

Authors: Corey Oses, Cormac Toher & Stefano 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

Nature Communications

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

Authors: Pranab Sarker†, Tyler J. Harrington†, Cormac Toher, Corey Oses, Mojtaba Samiee, Jon-Paul Maria, Donald W. Brenner, Kenneth S. Vecchio & Stefano Curtarolo
† 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

NPJ Computational Materials

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

Authors: Valentin Stanev, Corey Oses, Aaron Gilad Kusne, Efrain Rodriguez, Johnpierre Paglione, Stefano Curtarolo & Ichiro 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

Computational Materials Science

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

Authors: Eric Gossett, Cormac Toher, Corey Oses, Olexandr Isayev, Fleur Legrain, Frisco Rose, Eva Zurek, Jesús Carrete, Natalio Mingo, Alexander Tropsha & Stefano 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

Acta Crystallographica Section A

11 *AFLOW-SYM: platform for the complete, automatic and self-consistent symmetry analysis of crystals*
Acta Cryst. A **74**, 184–203 (2018)

Authors: David Hicks, Corey Oses, Eric Gossett, Geena Gomez, Richard H. Taylor, Cormac Toher, Michael J. Mehl, Ohad Levy & Stefano 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

2017

Inorganic Chemistry

10 *The structure and composition statistics of 6A binary and ternary structures*
Inorg. Chem. **57**(2), 653–667 (2017)

Authors: Alon Hever, Corey Oses, Stefano Curtarolo, Ohad Levy & Amir 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

Computational Materials Science

9

AFLUX: The LUX materials search API for the AFLOW data repositories
Comput. Mater. Sci. **137**, 362–370 (2017)

Authors: Frisco Rose, Cormac Toher, Eric Gossett, Corey Oses, Marco Buongiorno Nardelli, Marco Fornari & Stefano 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

Nature Communications

8

Universal Fragment Descriptors for Predicting Properties of Inorganic Crystals
Nat. Commun. **8**, 15679 (2017)

Authors: Olexandr Isayev†, Corey Oses†, Cormac Toher, Eric Gossett, Stefano Curtarolo & Alexander Tropsha

† 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

Physical Review Materials

7

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

Authors: Cormac Toher, Corey Oses, Jose J. Plata, David Hicks, Frisco Rose, Ohad Levy, Maarten de Jong, Mark Asta, Marco Fornari, Marco Buongiorno Nardelli & Stefano 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

Acta Materialia 6

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

Authors: Chandramouli Nyshadham, Corey Oses, Jacob E. Hansen, Ichiro Takeuchi, Stefano Curtarolo & Gus L. W. 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 $L1_2$ phase, which is in two-phase equilibrium with the fcc matrix. Inspired by this unexpected discovery of an $L1_2$ ternary phase, we performed a first-principles search through 2224 ternary metallic systems for analogous precipitate-hardening phases of the form $X_3[A_{0.5}, B_{0.5}]$, 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_3(Al, W) superalloy. They have a stable two-phase equilibrium with the host matrix within the concentration range $0 < x < 1$ ($X_3[A_x, B_{1-x}]$) 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

Science Advances 5

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

Authors: Stefano Sanvito, Corey Oses, Junkai Xue, Anurag Tiwari, Mario Žic, Thomas Archer, Pelin Tozman, Munuswamy Venkatesan, J. Michael D. Coey & Stefano 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_C, was estimated by a regression calibrated on the experimental T_C 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_2MnTi, which displays a remarkably high T_C in perfect agreement with the predictions, and Mn_2PtPd, 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

2016

Physical Review X 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: Ambroise van Roekeghem, Jesús Carrete, Corey Oses, Stefano Curtarolo & Natalio 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

Chemistry of Materials

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

Authors: Kesong Yang, Corey Oses & Stefano 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 ($ZnS_{1-x}Se_x$), a wide-gap oxide semiconductor ($Mg_xZn_{1-x}O$), and an iron alloy ($Fe_{1-x}Cu_x$), 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

2015

Computational Materials Science

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

Authors: Camilo E. Calderon, Jose J. Plata, Cormac Toher, Corey Oses, Ohad Levy, Marco Fornari, Amir Natan, Michael J. Mehl, Gus L. W. Hart, Marco Buongiorno Nardelli & Stefano 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

Chemistry of Materials

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

Authors: Olexandr Isayev, Denis Fourches, Eugene N. Muratov, Corey Oses, Kevin M. Rasch, Alexander Tropsha & Stefano 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

Book Publications

2019

Book Chapter 3 Automated computation of materials properties, *Materials Informatics: Methods, Tools and Applications*

Authors: Cormac Toher, Corey Oses & Stefano Curtarolo
Abstract: Materials informatics offers a promising pathway towards rational materials design, replacing the current trial-and-error approach and accelerating the development of new functional materials. Through the use of sophisticated data analysis techniques, underlying property trends can be identified, facilitating the formulation of new design rules. Such methods require large sets of consistently generated, programmatically accessible materials data. Computational materials design frameworks using standardized parameter sets are the ideal tools for producing such data. This work reviews the state-of-the-art in computational materials design, with a focus on these automated *ab-initio* frameworks. Features such as structural prototyping and automated error correction that enable rapid generation of large datasets are discussed, and the way in which integrated workflows can simplify the calculation of complex properties, such as thermal conductivity and mechanical stability, is demonstrated. The organization of large datasets composed of *ab-initio* calculations, and the tools that render them programmatically accessible for use in statistical learning applications, are also described. Finally, recent advances in leveraging existing data to predict novel functional materials, such as entropy stabilized ceramics, bulk metallic glasses, thermoelectrics, superalloys, and magnets, are surveyed.
URL: wiley.com/en-us/Materials+Informatics%3A+Methods%2C+Tools%2C+and+Applications-p-9783527802272

2018

Book Chapter 2 Machine learning and high-throughput approaches to magnetism, *Handbook of Materials Modeling. Volume 2 Applications: Current and Emerging Materials*

Authors: Stefano Sanvito, Mario Žic, James Nelson, Thomas Archer, Corey Oses & Stefano Curtarolo
Abstract: Magnetic materials have underpinned human civilization for at least one millennium and now find applications in the most diverse technologies, ranging from data storage, to energy production and delivery, to sensing. Such great diversity, associated to the fact that only a limited number of elements can sustain a magnetic order, makes magnetism rare and fascinating. The discovery of a new high-performance magnet is often a complex process, where serendipity plays an important role. Here we present a range of novel approaches to the discovery and design of new magnetic materials, which is rooted in high-throughput electronic structure theory and machine learning models. Such combination of methods has already demonstrated the ability of discovering ferromagnets with high Curie temperature at an unprecedented speed.
DOI: 10.1007/978-3-319-50257-1_108-1

Book Chapter 1 The AFLOW Fleet for Materials Discovery, *Handbook of Materials Modeling. Volume 1 Methods: Theory and Modeling*

Authors: Cormac Toher, Corey Oses, David Hicks, Eric Gossett, Frisco Rose, Pinku Nath, Demet Usanmaz, Denise C. Ford, Eric Perim, Camilo E. Calderon, Jose J. Plata, Yoav Lederer, Michal Jahnátek, Wahyu Setyawan, Shidong Wang, Junkai Xue, Kevin M. Rasch, Roman V. Chepulskii, Richard H. Taylor, Geena Gomez, Harvey Shi, Andrew R. Supka, Rabih Al Rahal Al Orabi, Priya Gopal, Frank T. Cerasoli, Laalitha Liyanage, Haihang Wang, Ilaria Siloi, Luis A. Agapito, Chandramouli Nyshadham, Gus L. W. Hart, Jesús Carrete, Fleur Legrain, Natalio Mingo, Eva Zurek, Olexandr Isayev, Alexander Tropsha, Stefano Sanvito, Robert M. Hanson, Ichiro Takeuchi, Michael J. Mehl, Aleksey N. Kolmogorov, Kesong Yang, Pino D'Amico, Arrigo Calzolari, Marcio Costa, Riccardo De Gennaro, Marco Buongiorno Nardelli, Marco Fornari, Ohad Levy & Stefano Curtarolo
Abstract: The traditional paradigm for materials discovery has been recently expanded to incorporate substantial data driven research. With the intent to accelerate the development and the deployment of new technologies, the AFLOW Fleet for computational materials design automates high-throughput first principles calculations, and provides tools for data verification and dissemination for a broad community of users. AFLOW incorporates different computational modules to robustly determine thermodynamic stability, electronic band structures, vibrational dispersions, thermo-mechanical properties and more. The AFLOW data repository is publicly accessible online at aflow.org, with more than 1.7 million materials entries and a panoply of queryable computed properties. Tools to programmatically search and process the data, as well as to perform online machine learning predictions, are also available.
DOI: 10.1007/978-3-319-42913-7_63-1

TEACHING EXPERIENCE

Teaching Assistant	Fall 2014–Spring 2015	ME 221: Structure and Properties of Solids, Duke University Department of Mechanical Engineering and Materials Science

Introduction to materials science and engineering, emphasizing the relationships between the structure of a solid and its properties. Atomic and molecular origins of electrical, mechanical, and chemical behavior are treated in some detail for metals, alloys, polymers, ceramics, glasses, and composite materials.

- Best Teaching Assistant Award, August 14, 2015

CERTIFICATIONS

Participant	June 11–14, 2019	CECAM (Centre Européen de Calcul Atomique et Moléculaire) Open Databases Integration for Materials Design (OPTiMaDe) Workshop at the École polytechnique fédérale de Lausanne (EPFL)
Graduate	June 25–29, 2018	Machine Learning Summer School (MLSS) at Duke University
Participant	June 11–15, 2018	CECAM (Centre Européen de Calcul Atomique et Moléculaire) Open Databases Integration for Materials Design (OPTiMaDe) Workshop at the École polytechnique fédérale de Lausanne (EPFL)
Graduate	September 26–29, 2017	*NextProf* Workshop at the University of Michigan
Graduate	January 7–16, 2015	Machine Learning Summer School (MLSS) at the University of Texas at Austin
Graduate	May 22–27, 2011	*The LeaderShape Institute* at Cornell University
Technician License	July 29, 2010	American Radio Relay League (ARRL) in Roselle, New Jersey

ACTIVITIES AND OUTREACH

Graduate Representative	2015–2018	Council of Presidents, Duke University Graduate School
Member	2014–Present	American Physical Society
Graduate Student Advisor	2009–2018	Society of Hispanic Professional Engineers, Duke University & Cornell University

Positions: Graduate Student Advisor, President, Corporate Vice President & Treasurer

Undergraduate Researcher	2011–2013	Brock Research Group, Cornell University
Distinguished Past Governor	2010–2013	Circle K, Cornell University

Positions: New York District Distinguished Past Governor, New York District Distinguished Past Treasurer & Restarting Chapter President at Cornell University

Member	2009–2013	Meinig Family Cornell National Scholars, Cornell Commitment
Mechanical Engineer	2009–2011	Cornell University Autonomous Flight Team, Cornell University

Constructed an autonomous plane with capabilities to navigate waypoints, survey areas, and retrieve visual information about the surfaces below as part of a team effort for AUVSI's (Association for Unmanned Vehicle Systems International) Student Unmanned Aerial Systems Competition.
Positions: Mechanical Engineer, Safety Officer & Systems Manager

President	2005–2009	Future Business Leaders of America, Bloomfield High School

Positions: President & General Manager of School Store

Membership Director	2005–2009	Key Club, Bloomfield High School

Positions: Membership Director & Activities Director

Retreat Team	2005–2009	Youth Group, Saint Thomas the Apostle Church

Positions: Retreat Team, Lead Role in *Stations of the Cross Performance* & Confirmation Class Instructor

President	2008–2009	Astronomy Club, Bloomfield High School
Member	2009	United Astronomy Clubs of New Jersey

Member	2009	New Jersey Astronomical Group, Montclair State University
Secretary	2006–2009	Model United Nations, Bloomfield High School
	Positions: Secretary & Treasurer	
Treasurer	2006–2009	Math Team, Bloomfield High School
Member	2006–2009	Science Club, Bloomfield High School
	Physics Club · Chemistry Club	
Athlete	2006–2009	Spring Track and Field, Bloomfield High School
	Javelin Junior Varsity Team	
Member	2006–2009	Weight Lifting Team, Bloomfield High School
Tutor	2006–2009	Tutor at the Library, Bloomfield High School
County Freeholder	2008	American Legion Jersey Boys State
	Positions: County Freeholder & City Councilman	
Member	2005–2008	Latin Club, Bloomfield High School
Member	2005–2006	Bowling Team, Bloomfield High School
Black belt	2002–2006	Tae Kwon Do, USMA in Clifton, New Jersey