COREY OSES

Ph.D. Candidate in Materials Science, Duke University

Personal Information · Objective · Education · Research · Teaching Experience · Work Experience and Skills · Activities and Outreach · Press and News Releases · Honors and Awards · Journal Publications · Book Publications

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.

EDUCATION

Ph.D. Candidate

2013–Present Duke University

GPA: 3.8/4.0 · Department: Mechanical Engineering and Materials Science
Thesis: *Advanced Techniques in High-Throughput Computational Materials Science*
Advisor: Stefano Curtarolo

Bachelor of Science

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*

RESEARCH

Duke University

2015–2018 Advanced Techniques in High-Throughput Computational Materials Science

Implemented algorithms for the analysis of partial charge, vibrational modes, and mechanical and thermodynamic stability. · Developed predictive models and novel materials discovery abstractions, such as Materials Cartography, toward the goal of rational materials design. · **Focus**: Full implementation of the AFLOW Superconductivity Library (ASL), which, given any material structure, will perform all necessary analyses needed for the calculation of the superconductivity critical temperature under the Allen-Dynes modified McMillan formulation in an automatic, high-throughput fashion.

- Completed Preliminary Defense — June 24, 2016.

Committee Members: Stefano Curtarolo, Cormac H. Toher, Laurens E. Howle & Gus L. W. Hart

2015–2017 **Fragment Descriptors for Predicting Property of Inorganic Crystals**

Duke University

Developed property-labeled fragments that demonstrate robust screening capabilities and design rule discovery in inorganic crystals. · Collaborative effort between UNC-Chapel Hill and Duke University.

- Presented at APS March Meeting 2017.
- Publication in Nat. Commun. (2017).

Advisor: Stefano Curtarolo

2014–2016 **Modeling Off-Stoichiometry Materials**

Duke University

Developed and implemented a robust framework for modeling off-stoichiometry and aperiodic materials in a high-throughput fashion. · Collaborative effort between UCSD and Duke University.

- Engineering Science Symposium Finalist, SHPE Conference 2016.
- Presented at APS March Meeting 2016.
- Publication in Chem. Mater. (2016).

Advisor: Stefano Curtarolo

2014 **Materials Cartography**

Duke University

Developed novel fingerprinting method for electronic properties of materials that enabled the construction of similarity maps. · Collaborative effort between UNC-Chapel Hill and Duke University.

- Presented at BYU Condensed Matter Physics Seminar — February 18, 2016.
- Presented at Duke MEMS Department Graduate Student Seminar — September 25, 2015.
- Presented at APS March Meeting 2015.
- Publication in Chem. Mater. (2015).

Advisor: Stefano Curtarolo

Fall 2012–Spring 2013 **Plume Propagation Simulation for Pulsed Laser Deposition**

Cornell University

Developed a three-dimensional Monte-Carlo simulation of the Pulsed Laser Deposition material growth technique used at the Cornell High Energy Synchrotron Source.

- Presented at NSF / AAAS / EHR Emerging Researchers National Conference 2014.
- Technical poster presentation, MRS / ASM / AVS / AReMS Meeting at NC State University — November 15, 2013.
- Technical Poster and Paper Finalist, SHPE Conference 2013.
- Best Presentation Award, Duke MEMS Department Retreat 2013.

Advisor: Joel Brock

Summer 2012 **Synchrotron Radiation Focusing Optics — Capillary Beam Stop Design**

Cornell High Energy Synchrotron Source

Designed a beam stop assembly to eliminate parasitic X-Ray beams and improve focusing capabilities of the ellipsoidal glass capillary optic.

- First Place in Nanoscience and Physics Research Presentation, NSF / AAAS / EHR Emerging Researchers National Conference 2013.
- Technical poster and research presentation, Cornell University LSAMP Research Symposium — August 7, 2012.

Advisors: Ernest Fontes & Rong Huang

Fall 2011–Spring 2012

Conductivity Behavior in Strontium Titanate

Cornell University

Verified a model that characterizes the conductivity of annealed Strontium Titanate samples. · Further investigated conductivity behavior of annealed Strontium Titanate samples under varying electric potentials.
Advisor: Joel Brock

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 Air Systems Competition.

- Served as team's safety officer and head systems manager, AUVSI Student Unmanned Air System (SUAS) 2010 Competition.
- Won a $1,000 grant, AUVSI Student Unmanned Air System (SUAS) 2010 Competition.

Advisor: Ashutosh Saxena

2009–2010

Meinig Family Cornell National Scholars

Cornell University

Collaborated with MFCNS, scholarship fund director, and the Cornell Alumni Association for the 2009–2010 annual research project, Academic Integrity, culminating with group presentation and discussion with relevant Cornell faculty and professors.
Advisor: Kristine M. DeLuca

Teaching Experience

Fall 2014–Spring 2015

ME 221: Structure and Properties of Solids, Duke University

Teaching Assistant

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, Spring 2015

Work Experience and Skills

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

Graduate — *January 2015* — Machine Learning Summer School at the University of Texas, Austin

Internship — *Summer 2013* — Cornell High Energy Synchrotron Source (BioSAXS on F2 and G Beamlines)
Supervisors: Richard Edward Gillilan & Ernest Fontes

Graduate — *May 2011* — *The LeaderShape Institute*

Student Employee — *Summer 2011* — ILR Budget Office, Cornell University
Supervisor: Renee Laree Monroe

Technician License — *July 2010* — American Radio Relay League (ARRL)

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

Activities and Outreach

Graduate Representative	*2015–Present*	Council of Presidents, Duke Graduate School
Member	*2014–Present*	American Physical Society
Graduate Student Advisor	*2009–Present*	Society of Hispanic Professional Engineers, Duke University & Cornell University **Positions**: Graduate Student Advisor, President, Corporate Vice President & Treasurer
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 **Positions**: Mechanical Engineer & Safety Officer
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

Press and News Releases

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! and Phys.org.

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

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

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

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

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.

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

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

https://research.duke.edu/molecular-tornado

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

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

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

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

New York Kiwanis	*February 2013*	*"New York Kiwanis Mid-Winter Conference 2013"* http://www.kiwanis-ny.org/1213/midyear.htm
New York Kiwanis	*June 2012*	*"K-Kids Show Talent for Fundraising"* http://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. http://www.kiwanis-ny.org/news/view_news.php?nid=618
Cornell University	*March 2011*	*"Undergraduate Student of the Month"* https://www.engineering.cornell.edu/diversity/about/honors/students/2011-03.cfm

HONORS AND AWARDS

Fellowship	*2013–2016*	Graduate Research Fellowship, National Science Foundation
Fellowship	*2013–2015*	Associate Fellow, The National GEM Consortium
City Citation	*March 21, 2013*	New York City Citation as Circle K Governor, Council Member Fernando Cabrera
Award	*October 8, 2011*	College Bowl Winner, 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
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

2017

In Preparation

12 *AFLOW Platform for Low-Temperature Thermodynamic Phase Stability Analyses*

Authors: Corey Oses, Eric Perim, Eric Gossett, Frisco Rose & Stefano Curtarolo

Abstract: Determination of thermodynamic stability plays a crucial role in any materials design initiative. We explore some of the analyses that are of particular importance to the high-throughput *ab-initio* community and present a new module for performing these calculations within the software platform AFLOW. Leveraging the AFLOW RESTful API, this module goes beyond the standard convex hull plot interface with tools and options that enable users to rapidly create and interact with thermodynamic stability data. In addition to the creation of fully functional documents, AFLOW Hull powers an online graphical interface available via the AFLOW Online Portal. We hope that the adoption of such rapid post-processing frameworks will lead to the development of novel materials descriptors and, correspondingly, new functional materials.

11 *Machine learning modeling of superconducting critical temperature*

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.

Submitted

arXiv: arxiv:1709.02727

10 *The structure and composition statistics of 6A binary and ternary structures*

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.

Submitted

arXiv: arxiv:1703.04497

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

Authors: Frisco Rose, Cormac H. 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.

Computational Materials Science

- This paper was selected for Editor's Choice.

DOI: 10.1016/j.commatsci.2017.04.036

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

Authors: Olexandr Isayev[†], Corey Oses[†], Cormac H. 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.

Nature Communications

DOI: 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: Cormac H. Toher, Corey Oses, Jose J. Plata, David J. 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.

Physical Review Materials

DOI: 10.1103/PhysRevMaterials.1.015401

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.

Acta Materialia

DOI: 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: Stefano Sanvito, Corey Oses, Junkai Xue, Anurag Tiwari, Mario Zic, Thomas Archer, Pelin Tozman, Munuswamy Venkatesan, J. Michael D. Coey & Stefano Curtarolo

Science Advances

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

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

Physical Review X

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

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.

Chemistry of Materials

DOI: 10.1021/acs.chemmater.6b01449

2015

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 H. 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.

Computational Materials Science

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

2017

In Preparation

1 Automated High-Throughput Computation of Material Properties, *Materials Informatics. Methods, Tools and Applications*

Authors: Cormac H. Toher, Corey Oses & Stefano Curtarolo