COREY OSES

Ph.D. Candidate in 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.

EDUCATION

2013–Present — Duke University

Ph.D. Candidate

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

2009–2013 — Cornell University

Bachelor of Science

GPA: 3.3/4.0 · Department: Applied and Engineering Physics
Thesis: *Plume Propagation Simulation for Pulsed Laser Deposition*
Advisor: Joel Brock

2005–2009 — Bloomfield High School

High School Diploma

GPA: 3.9/4.0 · *Graduated fifth in class of 428*

PRESS AND NEWS RELEASES

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

MRS Bulletin

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

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

UNC Eshelman School of Pharmacy

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

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

April 2017 — *"Computers Create Recipe for Two New Magnetic Materials"*

Duke University Pratt School of Engineering Research

- 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.

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

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

Computational Chemistry Highlights

- "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

January 2015 — *"Molecular Tornado"*

Duke University Research

research.duke.edu/molecular-tornado

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

Duke University

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

Duke University	*June 2014*	*"Pratt Profiles: Corey Oses"* pratt.duke.edu/graduate/diversity/pratt-profiles-corey-oses
New York Kiwanis	*February 2013*	*"New York Kiwanis Mid-Winter Conference 2013"* kiwanis-ny.org/1213/midyear.htm
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
Cornell University	*March 2011*	*"Undergraduate Student of the Month"* engineering.cornell.edu/diversity/about/honors/students/2011-03.cfm

Honors and Awards

Publication Award	*2018*	Editor's Choice, Publication in Comput. Mater. Sci., Elsevier
Award	*November 3, 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 4, 2016*	Presentation Finalist at the Engineering Science Symposium, SHPE National Conference
Award	*Spring 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, The National GEM Consortium
Award	*November 1, 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 2, 2013*	First Place in Nanoscience and Physics Research Presentation, NSF / AAAS / EHR Emerging Researchers National Conference
Award	*October 8, 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* Beta Delta Chapter	*Men of Principle* Award, Beta Theta Pi
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

TALKS / PRESENTATIONS

Poster Presentation	*2018*	Cloud-oriented computational phase diagrams with AFLOW-CHULL CECAM (Centre Européen de Calcul Atomique et Moléculaire) Open Databases Integration for Materials Design (OPTiMaDe) Workshop, Lausanne, Switzerland — June 11, 2018.
Contributed Talk	*2018*	Universal Fragment Descriptors for Predicting Properties of Inorganic Crystals **Contributed talk** at the Hopkins Extreme Materials Institute Mach Conference, Annapolis, Maryland — April 05, 2018. **Contributed talk** at the SHPE National Conference, Kansas City, Missouri — November 03, 2017. • Presentation Winner at the Engineering Science Symposium **Contributed talk** at the Duke University Chemistry Department Third Annual Graduate Research Symposium, Durham, North Carolina — October 09, 2017. **Contributed talk** at the American Physical Society March Meeting, New Orleans, Louisiana — March 14, 2017.

2018 — Advancements in Materials Informatics with AFLOW

Invited Talk

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

2016 — Modeling Off-Stoichiometric Materials with a High-Throughput, *Ab-Initio* Approach

Contributed Talk

Contributed talk at the SHPE National Conference, Seattle, Washington — November 04, 2016.

- Presentation Finalist at the Engineering Science Symposium

Contributed talk at the American Physical Society March Meeting, Baltimore, Maryland — March 16, 2016.

2016 — Advanced Techniques in High-Throughput Computational Materials Science

PhD Preliminary Exam

Duke University PhD Preliminary Exam, Durham, North Carolina — June 24, 2016.

- Passed preliminary examination

2016 — Materials Cartography: Representing and Mining Materials Space using Structural and Electronic Fingerprints

Invited Talk

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

2014 — Qualifying Exam: Computational Materials Science, Statistical Mechanics, and Applied Partial Differential Equations and Complex Variables

PhD Qualifying Exam

Duke University PhD Qualifying Exam, Durham, North Carolina — August 07, 2014.

- Passed qualifying examination

2014 — Plume Propagation Simulation for Pulsed Laser Deposition

Contributed Talk

Contributed talk at the NSF / AAAS / EHR Emerging Researchers National Conference, Washington, D.C. — February 22, 2014.
Poster presentation at the MRS / ASM / AVS / AReMS Meeting, North Carolina State University, Raleigh, North Carolina — November 15, 2013.
Poster presentation at the SHPE National Conference, Indianapolis, Indiana — November 01, 2013.

- Technical Poster and Paper Finalist at the Engineering Science Symposium

Poster presentation at the Duke Mechanical Engineering and Materials Science (MEMS) Department Annual Retreat, Durham, North Carolina — August 22, 2013.

- Best Presentation Award

2013 — Synchrotron Radiation Focusing Optics — Capillary Beam Stop Design

Contributed Talk

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

Poster presentation at the Cornell University Chapter of LSAMP Research Symposium, Ithaca, New York — August 07, 2012.

2010 — AEOLUS Unmanned Aerial Reconnaissance System by CU AIR

Group Presentation

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

2010 — Academic Integrity

Group Presentation

Meinig Family Cornell National Scholars Freshman Forum, Ithaca, New York — April 21, 2010.

BOOK PUBLICATIONS

2018

Submitted

3 Automated computation of materials properties, *Materials Informatics*

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.

arXiv: arxiv:1805.05309

Submitted

2 Machine learning and high-throughput approaches to magnetism, *to be determined*

Authors: Stefano Sanvito, Mario Zic, James Nelson, Thomas Archer, Corey Oses & Stefano Curtarolo

Abstract: Magnetic materials have underpinned human civilisation 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.

Submitted

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.

arXiv: arxiv:1712.00422

JOURNAL PUBLICATIONS

2018

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

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.

Submitted

arXiv: arxiv:1806.06901

15 *Autonomous data-driven materials design of inorganic compounds with AFLOW*

Authors: Corey Oses, Cormac Toher & Stefano Curtarolo

Abstract: The expansion of programmatically-accessible materials data has cultivated opportunities for data-driven approaches. Highly-automated frameworks like AFLOW 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.

Submitted

arXiv: arxiv:1803.05035

14 *Novel high-entropy high-hardness metal carbides discovered by entropy descriptors*

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

† contributed equally

Submitted

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.

NPJ Computational Materials

DOI: 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: 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.

Computational Materials Science

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

Acta Crystallographica Section A

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

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

Inorganic Chemistry

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

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

Computational Materials Science

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

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.

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 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.

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

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.

Science Advances

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

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.

Physical Review X

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.
DOI: 10.1021/acs.chemmater.6b01449

Chemistry of Materials

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 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

Computational Materials Science

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

Chemistry of Materials

TEACHING EXPERIENCE

	Fall 2014–Spring 2015	ME 221: Structure and Properties of Solids, Duke University Department of Mechanical Engineering and Materials Science
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`
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 Edward Gillilan & Ernest Fontes	
Internship	*Summer 2012*	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. **Supervisors**: Rong Huang & Ernest Fontes	
Student Employee	*Summer 2011*	ILR Budget Office, Cornell University
	Supervisor: Renee Laree Monroe	
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	

Certifications

Graduate	*September 2017*	*NextProf* Workshop at the University of Michigan
Graduate	*January 2015*	Machine Learning Summer School at the University of Texas at Austin
Graduate	*May 2011*	*The LeaderShape Institute*
Technician License	*July 2010*	American Radio Relay League (ARRL)

Activities and Outreach

Graduate Representative	*2015–Present*	Council of Presidents, Duke University 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	
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

	2009–2011	Cornell University Autonomous Flight Team, Cornell University
Mechanical Engineer	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