# COREY OSES

Materials Science, Duke University

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

### PERSONAL INFORMATION

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website coreyoses.com

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

arXiv: arxiv:1811.08464 Advisor: Stefano Curtarolo

B.Sc. 2009-2013 Cornell University

**Department**: Applied and Engineering Physics

Thesis: Plume Propagation Simulation for Pulsed Laser Deposition

Advisor: Joel Brock

### 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

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

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

properties

June 2017

**UNC** Eshelman School of Pharmacy "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

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

 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

"Materials fingerprints identified for informatics" MRS Bulletin April 2015

doi.org/10.1557/mrs.2015.76

Computational Chemistry Highlights

"Materials Cartography: Representing and Mining Materials Space Using January 2015

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 January 2015 Research

"Molecular Tornado"

research.duke.edu/molecular-tornado

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

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

ERN Conference	February 2013	"2013 Oral and Poster Presentation Award Winners"		
2013	new.emerging-researchers.org/2013-oral-and-poster-presentation-winners			
HONORS AND A	WARDS			
Publication Award	2018	Editor's Choice, Publication in Comput. Mater. Sci., Elsevier		
Publication Award	2017	Editor's Choice, Publication in Comput. Mater. Sci., Elsevier		
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		
Award	August 22, 2013	Best Presentation Award at the MEMS Departmental Retreat, Duke University Department of Mechanical Engineering and Materials Science		
Award	March 02, 2013	First Place in Nanoscience and Physics Research Presentation, NSF / AAAS / EHR Emerging Researchers National Conference		
Scholarship	2011–2013	Shell Incentive Fund Scholarship		
Scholarship	2010 & 2011	Xerox Corporation Scholarship		
Scholarship	2010 & 2011	Intel Academic Award		
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		
TALKS / PRESENTATIONS				
Contributed Talk		l Fragment Descriptors for Predicting Properties of Inorganic Crystals		
	Contributed talk at the International Association for Computational Mechanics (IACM) 13 <sup>th</sup> World Congress in Computational Mechanics (WCCM), New York City, New York — July 23, 2018.  Contributed talk at the Hopkins Extreme Materials Institute Mach Conference, Annapolis, Maryland — April 05, 2018.  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.			
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

2016

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

Advancements in Materials Informatics with AFLOW

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

Invited talk at the Fritz-Haber-Institut der Max-Planck-Gesellschaft Theory Department Seminar, Berlin,

Invited talk at the Humboldt University of Berlin Physics Department Seminar, Berlin, Germany — January

Design (OPTiMaDe) Workshop, Lausanne, Switzerland — June 11, 2018.

Germany — January 18, 2018.

16, 2018.

Invited Talk

Invited Talk

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

**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.

Contributed Talk

2015 Plume Propagation Simulation for Pulsed Laser Deposition

**Poster presentation** at the University of Texas at Austin Machine Learning Summer School (MLSS), Austin, Texas — January 12, 2015.

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

• Best Presentation Award

Contributed Talk

2013 Synchrotron Radiation Focusing Optics — Capillary Beam Stop Design

**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.

### JOURNAL PUBLICATIONS

### 2018

Submitted

18 Coordination corrected ab initio formation enthalpies

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

arXiv: arxiv:1811.08952

Submitted

17 AFLOW-QHA3P: Robust and automated method to compute thermodynamic properties of solids

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

**arXiv**: arxiv:1807.04669

Journal of Chemical Information and Modeling AFLOW-CHULL: Cloud-oriented platform for autonomous phase stability analysis J. Chem. Inf. Model. in press (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 DOI: 10.1021/acs.jcim.8b00393

Data-driven design of inorganic materials with the Automatic Flow Framework for

MRS Bulletin

Materials Discovery

MRS Bull. **43**(9), 670–675 (2018)

Authors: Corey Oses, Cormac Toher & Stefano Curtarolo

**DOI**: 10.1557/mrs.2018.207

15

Nature Communications Novel high-entropy high-hardness metal carbides discovered by entropy descriptors

Note Commune 9, 4000 (2018)

Nat. Commun. **9**, 4980 (2018)

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

† contributed equally

**DOI**: 10.1038/s41467-018-07160-7

NPI Computational Materials

Machine learning modeling of superconducting critical temperature 13

NPJ Comput. Mater. 4(29) (2018)

Authors: Valentin Staney, Corey Oses, Aaron Gilad Kusne, Efrain Rodriguez, Johnpierre Paglione, Stefano

Curtarolo & Ichiro Takeuchi DOI: 10.1038/s41524-018-0085-8

Computational Materials Science 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

• This paper was selected for Editor's Choice.

DOI: 10.1016/j.commatsci.2018.03.075

AFLOW-SYM: platform for the complete, automatic and self-consistent symmetry

11 analysis of crystals

Acta Cryst. A 74, 184–203 (2018)

Crystallographica Section A

Authors: David Hicks, Corey Oses, Eric Gossett, Geena Gomez, Richard H. Taylor, Cormac Toher, Michael

J. Mehl, Ohad Levy & Stefano Curtarolo DOI: 10.1107/S2053273318003066

2017

Acta

Inorganic Chemistry

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

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

DOI: 10.1021/acs.inorgchem.7b02462

Computational Materials Science 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

• This paper was selected for Editor's Choice.

DOI: 10.1016/j.commatsci.2017.04.036

Nature Communications

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

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

† contributed equally DOI: 10.1038/ncomms15679

Combining the AFLOW GIBBS and elastic Libraries to efficiently and robustly screening

7 thermomechanical properties of solids Physical Review Materials Phys. Rev. Mater. 1, 015401 (2017)

6

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

DOI: 10.1103/PhysRevMaterials.1.015401

Acta Materialia

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

DOI: 10.1016/j.actamat.2016.09.017

Science Advances

Accelerated Discovery of New Magnets in the Heusler Alloy Family 5 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

DOI: 10.1126/sciadv.1602241

2016

High-Throughput Computation of Thermal Conductivity of High-Temperature Solid

Physical Review X

4

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

**DOI**: 10.1103/PhysRevX.6.041061

Chemistry of Materials 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

**DOI**: 10.1021/acs.chemmater.6b01449

### 2015

Computational Materials Science *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

• This paper was selected for Editor's Choice.

DOI: 10.1016/j.commatsci.2015.07.019

Materials Cartography: Representing and Mining Materials Space Using Structural

Chemistry of Materials *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

• This paper was selected for Editor's Choice.

DOI: 10.1021/cm503507h

### BOOK PUBLICATIONS

### 2018

Submitted

3 Automated computation of materials properties

Authors: Cormac Toher, Corey Oses & Stefano Curtarolo

arXiv: arxiv:1805.05309

Book Chapter

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 **DOI**: 10.1007/978-3-319-50257-1\_108-1

Book Chapter

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

**DOI**: 10.1007/978-3-319-42913-7\_63-1

### TEACHING EXPERIENCE

Teaching Assistant

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

• Best Teaching Assistant Award, August 14, 2015

### WORK EXPERIENCE

Internship	Summer 2013	Cornell High Energy Synchrotron Source (BioSAXS on F2 and G Beamlines)	
	Supervisors: Richard E. Gillilan & Ernest Fontes		
Internship	Summer 2012	Cornell High Energy Synchrotron Source (Capillary Optics Group)	
	Supervisors: Rong Huang & Ernest Fontes		
Office Assistant	Summer 2011	ILR Budget Office, Cornell University	
	Supervisor: Renee Monroe Cook		

## CERTIFICATIONS

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	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