# COREY OSES

Ph.D. Candidate in Materials Science, Duke University

#### PERSONAL INFORMATION

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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 Department: Applied and Engineering Physics

Science Thesis: Plume Propagation Simulation for Pulsed Laser Deposition

Advisor: Joel Brock

#### PRESS AND NEWS RELEASES

August 2017 "Universal fragment descriptor predicts materials

MRS Bulletin properties"

https://www.cambridge.org/core/journals/mrs-bulletin/news/universal-fragment-

descriptor-predicts-materials-properties

UNC Eshelman

"Breakthrough Tool Predicts Properties of Theoretical Materials, Finds New Uses for Current Ones"

School of

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

Pharmacy http://pharmacy.unc.edu/news/2017/06/06/breakthrough-tool-predicts-properties-

theoretical-materials-finds-new-uses-current-ones/

Duke University

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.

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

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

Computational
Chemistry
•

Highlights A

• "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 January 2015 "Molecular Tornado"

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

Duke University	October 2014 https://gradscho	"Competing for NSF Fellowships: Advice from a Current Fellow"  pol.duke.edu/professional-development/blog/competing-nsf-	
	fellowships-advice-current-fellow		
Duke University	June 2014 http://pratt.duk	"Pratt Profiles: Corey Oses" e.edu/graduate/diversity/pratt-profiles-corey-oses	
New York Kiwanis	February 2013 http://www.kiw	"New York Kiwanis Mid-Winter Conference 2013" vanis-ny.org/1213/midyear.htm	
New York Kiwanis	June 2012 http://patch.com	"K-Kids Show Talent for Fundraising"  n/new-york/eastmeadow/k-kids-show-talent-for-fundraising	
New York Kiwanis	March 2012 http://www.kiw	"Past Circle K Governors Help Celebrate 50th Convention" vanis-ny.org/news/view_news.php?nid=618	
Cornell University	March 2011 https://www.en. 03.cfm	"Undergraduate Student of the Month" gineering.cornell.edu/diversity/about/honors/students/2011-	
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
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
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	Superintendent's Bengal Pride Award for Excellence in Academics and Citizenship
Scholarship	2009	Good Citizen Award, The Daughters of the American Revolution
Honor	2008–2009	National Honor Society

# TALKS/PRESENTATIONS

	Cloud-oriented computational phase diagrams with
	AFLOW-CHULL
Poster Presentation	CECAM (Centre Européen de Calcul Atomique et Moléculaire) Open Databases Integration for Materials Design (OPTiMaDe) Workshop, Lausanne, Switzerland —
	June 11, 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.

#### Contributed Talk

• 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.

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

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

#### Contributed Talk

• Presentation Finalist at the Engineering Science Symposium

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

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

**Invited talk** at the Brigham Young University Condensed Matter Physics Seminar, Provo, Utah — February 18, 2016.

Invited Talk

Contributed talk at the Duke Mechanical Engineering and Materials Science (MEMS)
Department Graduate Student Seminar, Durham, North Carolina — September 25,

**Contributed talk** at the American Physical Society March Meeting, San Antonio, Texas — March 02, 2015.

Plume Propagation Simulation for Pulsed Laser Deposition

**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.

Contributed Talk

Contributed Talk

**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

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.

#### BOOK PUBLICATIONS

## 2018

Automated computation of materials properties, *Materials Informatics* 

Submitted

Submitted

Authors: Cormac Toher, Corey Oses & Stefano Curtarolo arXiv: arxiv:1805.05309

Madaina 1

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

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

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

arXiv: arxiv:1712.00422

Submitted

JOURNAL PUBLICATIONS

2018

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

Submitted

**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

arXiv: arxiv:1806.06901

Autonomous data-driven materials design of inorganic compounds with AFLOW

Submitted

**Authors:** Corey Oses, Cormac Toher & Stefano Curtarolo arXiv: arxiv:1803.05035

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

Submitted

**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 <sup>†</sup> contributed equally

NPJ Computational Materials Machine learning modeling of superconducting critical temperature NPJ Comput. Mater. in press (2018)

**Authors**: Valentin Stanev, Corey Oses, Aaron Gilad Kusne, Efrain Rodriguez, Johnpierre Paglione, Stefano Curtarolo & Ichiro Takeuchi arXiv: arxiv:1709.02727

AFLOW-ML: A RESTful API for machine-learning prediction of materials properties

Comput. Mater. Sci. 152, 134–145 (2018)

Computational Materials Science

12

**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 analysis of crystals

Crystallographica Section A

Acta

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

**DOI**: 10.1107/S2053273318003066

2017

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

Inorganic Chemistry

Inorg. Chem. 57(2), 653-667 (2017)

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

**DOI**: 10.1021/acs.inorgchem.7b02462

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

Computational Materials Science

**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

Universal Fragment Descriptors for Predicting Properties of Inorganic

8 Crystals

Nature

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

7 robustly screening thermomechanical properties of solids

Physical Review Materials

Communications

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

DOI: 10.1103/PhysRevMaterials.1.015401

A Computational High-Throughput Search for New Ternary

6 Superalloys

Curtarolo

Acta Mater. 122, 438–447 (2017)

Acta Materialia

**Authors**: Chandramouli Nyshadham, Corey Oses, Jacob E. Hansen, Ichiro Takeuchi, Stefano Curtarolo & Gus L. W. Hart

**DOI**: 10.1016/j.actamat.2016.09.017

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

Science Advances

Physical Review

**Authors**: Stefano Sanvito, Corey Oses, Junkai Xue, Anurag Tiwari, Mario Zic, 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-

4 Temperature Solid Phases: The Case of Oxide and Fluoride Perovskites Phys. Rev. X **6**(4), 041061 (2016)

X

3

**Authors**: Ambroise van Roekeghem, Jesús Carrete, Corey Oses, Stefano Curtarolo & Natalio Mingo

DOI: 10.1103/PhysRevX.6.041061

Modeling Off-Stoichiometry Materials with a High-Throughput Ab-

Chemistry of Materials Initio Approach
Chem. Mater. **28**(18), 6484–6492 (2016)

Authors: Kesong Yang, Corey Oses & Stefano Curtarolo

DOI: 10.1021/acs.chemmater.6b01449

## 2015

The AFLOW Standard for High-Throughput Materials Science

2 *Calculations* 

Comput. Mater. Sci. 108A, 233–238 (2015)

Computational Materials Science

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

1 Using Structural and Electronic Fingerprints

Chem. Mater. 27(3), 735–743 (2015)

Chemistry of Materials

**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

#### TEACHING EXPERIENCE

Teaching Assistant

Fall 2014–
Spring 2015

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

• Best Teaching Assistant Award, Spring 2015

#### WORK EXPERIENCE

Summer 2013 Cornell High Energy Synchrotron Source (BioSAXS on

*Internship* F2 and G Beamlines)

Supervisors: Richard Edward Gillilan & Ernest Fontes

Internship Summer 2012 Cornell High Energy Synchrotron Source

**Supervisors**: Rong Huang & Ernest Fontes

#### CERTIFICATIONS

Graduate September 2017 NextProf Workshop at the University of Michigan

Graduate January 2015 Machine Learning Summer School at the University of

Texas, Austin

Graduate May 2011 The LeaderShape Institute

Technician
License

July 2010 American Radio Relay League (ARRL)

## ACTIVITIES AND OUTREACH

Graduate Council of Presidents, Duke University Graduate

Representative School

Member	2014–Present	American Physical Society
Graduate Student Advisor	2009–Present  Positions: Gradua	Society of Hispanic Professional Engineers, Duke University & Cornell University ate Student Advisor, President, Corporate Vice President & Treasurer
Distinguished Past Governor		Circle K, Cornell University  York District Distinguished Past Governor, New York District St Treasurer & Restarting Chapter President at Cornell University
Undergraduate Researcher	Fall 2011– Spring 2013	Brock Research Group, Cornell University
Mechanical Engineer	2009–2011  Positions: Mecha:	Cornell University Autonomous Flight Team, Cornell University nical Engineer, Safety Officer & Systems Manager