## 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

email corey.oses@duke.edu phone (W) +1 (919) 684 1553

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

ProQuest: link 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 November 2018 "Disordered Materials Could Be Hardest, Most Heat-Tolerant Ever"

Pratt School of Engineering

 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

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

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

properties

UNC Eshelman June 2017

School of Pharmacy

New Uses for Current Ones"
 This press release is featured on AAAS EurekAlert!, Phys.org, and ScienceDaily.

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

new-uses-current-ones/

Duke University

Pratt School of

Engineering

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

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

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

MRS Bulletin April 2015 "Materials fingerprints identified for informatics"

doi.org/10.1557/mrs.2015.76

Computational Chemistry

Highlights

nal January 2015

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

"Breakthrough Tool Predicts Properties of Theoretical Materials, Finds

 "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 "Molecular Tornado"

Research

research.duke.edu/molecular-tornado

Duke University

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

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

"2013 Oral and Poster Presentation Award Winners" ERN Conference February 2013 2013 new.emerging-researchers.org/2013-oral-and-poster-presentation-winners

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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

Invited Seminar 2019 AFLOW: Integrated infrastructure for computational materials discovery

> Co-Presenters: Cormac Toher, David Hicks, Eric Gossett, Marco Esters, Max J. Brenner & Stefano Curtarolo Invited seminar at the University of Pennsylvania AFLOW Full-Day Workshop, Philadelphia, Pennsylvania — May 03, 2019.

> Invited seminar at the North Carolina State University AFLOW Full-Day Workshop, Raleigh, North Carolina — March 12, 2019.

Invited seminar at the Carnegie Mellon University AFLOW Full-Day Workshop, Pittsburgh, Pennsylvania — January 21, 2019.

Invited seminar at the NIST/Moore Foundation/University of Maryland Machine Learning for Materials Research Bootcamp 2018 & Workshop on Machine Learning Quantum Materials, Institute for Bioscience & Biotechnology Research in Gaithersburg, Maryland — August 02, 2018.

Contributed Talk Cloud-oriented computational phase diagrams with AFLOW-CHULL

> Contributed talk at the American Physical Society March Meeting, Boston, Massachusetts — March 07, 2019. Poster presentation at the CECAM (Centre Européen de Calcul Atomique et Moléculaire) Open Databases Integration for Materials Design (OPTiMaDe) Workshop, Lausanne, Switzerland — June 11, 2018.

Invited Talk Going Off-Stoichiometry: Challenging Traditional Materials Discovery

Naval Research Laboratory Center for Computational Materials Science Seminar, Washington, D.C. —

January 09, 2019.

Contributed Talk Universal Fragment Descriptors for Predicting Properties of Inorganic Crystals

> Contributed talk at the International Association for Computational Mechanics (IACM) 13th 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.

Invited Talk 2018 Advancements in Materials Informatics with AFLOW

 $\textbf{Invited talk} \text{ at the Fritz-Haber-Institut der Max-Planck-Gesellschaft Theory Department Seminar, Berlin, and the properties of the$ 

Germany — January 18, 2018.

16, 2018.

Contributed Talk

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

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

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

2019

Submitted 21 Metallic glasses for biodegradable implants

Authors: Denise C. Ford, David Hicks, Corey Oses, Cormac Toher & Stefano Curtarolo

**arXiv**: arxiv:1902.00485

Submitted

Predicting Superhard Materials via a Machine Learning Informed Evolutionary Structure Search

Authors: Patrick Avery, Xiaoyu Wang, Eva Zurek, Davide M. Proserpio, Cormac Toher, Corey Oses, Eric Gossett & Stefano Curtarolo

NPJ Computational Materials *Unavoidable disorder and entropy in multi-component systems* 

NPJ Comput. Mater. in press (2019)

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

arXiv: arxiv:1906.01085

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

Physical Review Materials 18 of solids

Phys. Rev. Mater. in press (2019)

Authors: Pinku Nath, Demet Usanmaz, David Hicks, Corey Oses, Marco Fornari, Marco Buongiorno

Nardelli, Cormac Toher & Stefano Curtarolo

arXiv: arxiv:1807.04669

NPI Computational Materials

Coordination corrected ab initio formation enthalpies 17

NPJ Comput. Mater. 5(59) (2019)

Authors: Rico Friedrich, Demet Usanmaz, Corey Oses, Andrew R. Supka, Marco Fornari, Marco Buongiorno

Nardelli, Cormac Toher & Stefano Curtarolo

DOI: 10.1038/s41524-019-0192-1

2018

Journal of Chemical Information and Modeling

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

Authors: Corey Oses, Eric Gossett, David Hicks, Frisco Rose, Michael J. Mehl, Eric Perim, Ichiro Takeuchi, Stefano Sanvito, Matthias Scheffler, Yoav Lederer, Ohad Levy, Cormac Toher & Stefano Curtarolo

DOI: 10.1021/acs.jcim.8b00393

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

MRS Bulletin 15 Materials Discovery

MRS Bull. 43(9), 670-675 (2018)

Authors: Corey Oses, Cormac Toher & Stefano Curtarolo

DOI: 10.1557/mrs.2018.207

Nature

Communications

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

14 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

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

Authors: Valentin Stanev, 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

13

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

8 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

7

† contributed equally **DOI**: 10.1038/ncomms15679

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

Physical Review Materials 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

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

Physical Review X

Accelerated Discovery of New Magnets in the Heusler Alloy Family

Sci. Adv. 3(4), e1602241 (2017)

Authors: Stefano Sanvito, Corey Oses, Junkai Xue, Anurag Tiwari, Mario Žic, Thomas Archer, Pelin Tozman,

Munuswamy Venkatesan, J. Michael D. Coey & Stefano Curtarolo

**DOI**: 10.1126/sciadv.1602241

2016

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

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 1
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

2019
Submitted

3 Automated computation of materials properties

Authors: Cormac Toher, Corey Oses & Stefano Curtarolo

arXiv: arxiv:1805.05309

#### 2018

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

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

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

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

Authors: Cormac Toher, Corey Oses, David Hicks, Eric Gossett, Frisco Rose, Pinku Nath, Demet Usanmaz, Denise C. Ford, Eric Perim, Camilo E. Calderon, Jose J. Plata, Yoav Lederer, Michal Jahnátek, Wahyu Setyawan, Shidong Wang, Junkai Xue, Kevin M. Rasch, Roman V. Chepulskii, Richard H. Taylor, Geena Gomez, Harvey Shi, Andrew R. Supka, Rabih Al Rahal Al Orabi, Priya Gopal, Frank T. Cerasoli, Laalitha Liyanage, Haihang Wang, Ilaria Siloi, Luis A. Agapito, Chandramouli Nyshadham, Gus L. W. Hart, Jesús Carrete, Fleur Legrain, Natalio Mingo, Eva Zurek, Olexandr Isayev, Alexander Tropsha, Stefano Sanvito, Robert M. Hanson, Ichiro Takeuchi, Michael J. Mehl, Aleksey N. Kolmogorov, Kesong Yang, Pino D'Amico, Arrigo Calzolari, Marcio Costa, Riccardo De Gennaro, Marco Buongiorno Nardelli, Marco Fornari, Ohad Levy & Stefano Curtarolo

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

Supervisor: Renee Monroe Cook

### 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					
internentip	Summer 2010	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					

#### CERTIFICATIONS

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