### 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
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

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

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-pharmacy.unc.edu/news/2017/06/06/breakthrough-tool-predicts-properties-theoretical-materials-finds-pharmacy.unc.edu/news/2017/06/06/breakthrough-tool-predicts-properties-theoretical-materials-finds-pharmacy.unc.edu/news/2017/06/06/breakthrough-tool-predicts-properties-theoretical-materials-finds-pharmacy.unc.edu/news/2017/06/06/breakthrough-tool-predicts-properties-theoretical-materials-finds-pharmacy.unc.edu/news/2017/06/06/breakthrough-tool-predicts-properties-theoretical-materials-finds-pharmacy.unc.edu/news/2017/06/06/breakthrough-tool-predicts-properties-theoretical-materials-finds-pharmacy.unc.edu/news/2017/06/06/breakthrough-tool-predicts-properties-theoretical-materials-finds-pharmacy.unc.edu/news/2017/06/06/breakthrough-tool-pharmacy.unc.edu/news/2017/0

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 January 2015

"Materials Cartography: Representing and Mining Materials Space Using

Structural and Electronic Fingerprints"

• "This paper is a *tour de force* for computational materials science" — Prof. Alán Aspuru-Guzik, Harvard University.

 $compchem highlights.org/2015/01/materials\text{-}cartography\text{-}representing\text{-}and.html}$ 

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"

 ${\it Graduate School} \qquad {\it gradschool.} \\ {\it duke.edu/professional-development/blog/competing-nsf-fellowships-advice-current-fell$ 

ERN Conference	February 2013	"2013 Oral and Poster Presentation Award Winners"
2013	new.emerging-resear	chers.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
Inonea Semma	2017	ATLOW. Integrated infrastructure for computational materials discovery

Co-Presenters: Cormac Toher, David Hicks & Eric Gossett

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 & Biotcamp 2018 of Child probability of Maryland Associated 2, 2018

Biotechnology Research in Gaithersburg, Maryland — August 02, 2018.

Invited Talk 2019 Going Off-Stoichiometry: Challenging Traditional Materials Discovery

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

January 09, 2019.

Contributed Talk 2018 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.

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.

Invited Talk 2018 Advancements in Materials Informatics with AFLOW

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

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

21 Metallic glasses for biodegradable implants

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

arXiv: arxiv:1902.00485

Submitted

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

Submitted 19 The Unavoidable Disorder

Authors: Cormac Toher, Corey Oses & Stefano Curtarolo

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

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

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

Novel high-entropy high-hardness metal carbides discovered by entropy descriptors Nat. Commun. 9, 4980 (2018)

Communications

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

NPJ Computational Materials

Machine learning modeling of superconducting critical temperature 13

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 12 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 Crystallographica Acta Cryst. A 74, 184–203 (2018)

9

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

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 Phys. Rev. Mater. 1, 015401 (2017) Materials 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 A Computational High-Throughput Search for New Ternary Superalloys

Acta Materialia

6 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

Phases: The Case of Oxide and Fluoride Perovskites Physical Review X 4 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 2 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 and Electronic Fingerprints

Chemistry of Materials

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

1

BOOK PUBLICATIONS

2019

Submitted Automated computation of materials properties

Authors: Cormac Toher, Corey Oses & Stefano Curtarolo

arXiv: arxiv:1805.05309

2018

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

5

# 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

### TEACHING EXPERIENCE

Teaching Assistant Fall 2014–Spring ME 221: Structure and Properties of Solids, Duke University

2015 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