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-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 AFLOW: Integrated infrastructure for computational materials discovery 2019

> 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.

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

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.

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.

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

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 18 of solids

Materials 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

NPJ Computational Materials Coordination corrected ab initio formation enthalpies

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

110

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2018

Journal of Chemical Information and Modeling AFLOW-CHULL: Cloud-oriented platform for autonomous phase stability analysis 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 Nat. Commun. **9**, 4980 (2018)

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

† contributed equally

13

DOI: 10.1038/s41467-018-07160-7

NPJ 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

Acta Crystallographica 11 analysis of crystals
Acts Cryst A 74, 184, 203 (2018)

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

Inorganic Chemistry

Section A

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

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[†], Corey Oses[†], 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

Physical Review Materials 7 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

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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

Chemistry of

Materials

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

1 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

TEACHING EXPERIENCE

Teaching Assistant

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

- Det Techine Assistant Assess 14, 2015

• 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

CECAM (Centre Européen de Calcul Atomique et Moléculaire)

Participant June 11–14, 2019 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

CECAM (Centre Européen de Calcul Atomique et Moléculaire)

Participant June 11–15, 2018 Open Databases Integration for Materials Design (OPTiMaDe)

Workshop at the École polytechnique fédérale de Lausanne (EPFL)

Graduate January 7–16, Machine Learning Summer School (MLSS) at the University of Texas

2015 at Austin

Graduate May 22–27, 2011 The Leader Shape Institute at Cornell University

Technician License July 29, 2010 American Radio Relay League (ARRL) in Roselle, New Jersey