COREY OSES

Materials Science, Duke University

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

PERSONAL INFORMATION

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

website coreyoses.com

WORK EXPERIENCE

Postdoctoral Fellow 2018-present **Duke University**

Supervisor: Stefano Curtarolo

Cornell High Energy Synchrotron Source (BioSAXS on F2 and G Internship Summer 2013

Beamlines)

Supervisors: Richard E. Gillilan & Ernest Fontes

Cornell High Energy Synchrotron Source (Capillary Optics Group) Internship Summer 2012

Supervisors: Rong Huang & Ernest Fontes

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

pratt.duke.edu/about/news/chaotic-carbides

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.

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

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

properties

UNC Eshelman

June 2017 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

April 2017

"Computers Create Recipe for Two New Magnetic Materials"

Pratt School of

Engineering

• 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 • "This paper is a t University.	"Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints" our de force for computational materials science" — Prof. Alán Aspuru-Guzik, Harvard	
	$compchem highlights.org/2015/01/materials\hbox{-}cartography\hbox{-}representing\hbox{-}and.html$		
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	grads chool. duke. edu/professional-development/blog/competing-nsf-fellow ships-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		
ONORS AND A	AWARDS		

Η

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, Marco Esters, Eric Gossett, Max J. Brenner & Stefano Curtarolo Invited seminar at the NIST/Moore Foundation/University of Maryland Machine Learning for Materials Research Bootcamp 2019 & Workshop on Machine Learning Quantum Materials, Institute for Bioscience & Biotechnology Research in Gaithersburg, Maryland — August 05, 2019.

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 2019 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

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

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

Acta Materialia

Metallic glasses for biodegradable implants
Acta Mater. **176**, 297–305 (2019)

Authors: Denise C. Ford, David Hicks, Corey Oses, Cormac Toher & Stefano Curtarolo DOI: 10.1016/j.actamat.2019.07.008

Predicting Superhard Materials via a Machine Learning Informed Evolutionary Structure Search NPI Computational 20 NPJ Comput. Mater. 5, 89 (2019) Materials Authors: Patrick Avery, Xiaoyu Wang, Corey Oses, Eric Gossett, Davide M. Proserpio, Cormac Toher, Stefano Curtarolo & Eva Zurek DOI: 10.1038/s41524-019-0226-8 *Unavoidable disorder and entropy in multi-component systems* NPJ Computational 19 NPJ Comput. Mater. 5, 69 (2019) Materials Authors: Cormac Toher, Corey Oses, David Hicks & Stefano Curtarolo **DOI**: 10.1038/s41524-019-0206-z Coordination corrected ab initio formation enthalpies NPI Computational 18 NPJ Comput. Mater. 5, 59 (2019) Materials 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 AFLOW-QHA3P: Robust and automated method to compute thermodynamic properties Physical Review 17 Materials Phys. Rev. Mater. 3, 073801 (2019) Authors: Pinku Nath, Demet Usanmaz, David Hicks, Corey Oses, Marco Fornari, Marco Buongiorno Nardelli, Cormac Toher & Stefano Curtarolo DOI: 10.1103/PhysRevMaterials.3.073801 2018 AFLOW-CHULL: Cloud-oriented platform for autonomous phase stability analysis Journal of Chemical 16 J. Chem. Inf. Model. 58(12), 2477–2490 (2018) Information and Authors: Corey Oses, Eric Gossett, David Hicks, Frisco Rose, Michael J. Mehl, Eric Perim, Ichiro Takeuchi, Modeling 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 Novel high-entropy high-hardness metal carbides discovered by entropy descriptors Nature 14 Nat. Commun. 9, 4980 (2018) Communications Authors: Pranab Sarker[†], Tyler Harrington[†], 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 Machine learning modeling of superconducting critical temperature NPJ Computational 13

Materials

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 analysis of crystals Acta 11 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 The structure and composition statistics of 6A binary and ternary structures Inorganic 10 Inorg. Chem. 57(2), 653-667 (2017) Chemistry 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 9 Computational Comput. Mater. Sci. 137, 362–370 (2017) 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 Crystals Nature Nat. Commun. 8, 15679 (2017) Communications 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 7 Physical Review thermomechanical properties of solids Materials 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 A Computational High-Throughput Search for New Ternary Superalloys Acta Materialia 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 Accelerated Discovery of New Magnets in the Heusler Alloy Family 5 Science Advances 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 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 Modeling Off-Stoichiometry Materials with a High-Throughput Ab-Initio Approach Chemistry of 3 Chem. Mater. **28**(18), 6484–6492 (2016)

2015

Materials

Authors: Kesong Yang, Corey Oses & Stefano Curtarolo

DOI: 10.1021/acs.chemmater.6b01449

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 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

Book Chapter

Materials

Automated computation of materials properties, *Materials Informatics: Methods, Tools and Applications*, **in press**

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

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
2015 Department of Mechanical Engineering and Materials Science

• Best Teaching Assistant Award, August 14, 2015

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 May 22–27, 2011 The LeaderShape Institute at Cornell University

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