## COREY OSES

Materials Science, Duke University

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

PERSONAL INFORMATION

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

website coreyoses.com

WORK EXPERIENCE

Postdoctoral Fellow 2018–present Duke University

Supervisor: Stefano Curtarolo

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

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: search.proquest.com/docview/2172402640?pq-origsite=gscholar

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

ber 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-predicts-ma

properties

UNC Eshelman School of Pharmacy June 2017

"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/2017/06/06/06/breakthrough-tool-pharmacy.unc.edu/news/2017/06/06/breakthrough-tool-pharmacy.unc.edu/news/201

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	"Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints"	
		• "This paper is a <i>tour de force</i> for computational materials science" — Prof. Alán Aspuru-Guzik, Harvard University.		
		compchemhighlights.	org/2015/01/materials-cartography-representing-and.html	
	Duke University Research	January 2015 research.duke.edu/m	"Molecular Tornado"  olecular-tornado	
	Duke University Graduate School	October 2014 gradschool.duke.edu/	"Competing for NSF Fellowships: Advice from a Current Fellow"  /professional-development/blog/competing-nsf-fellowships-advice-current-fellow	
	ERN Conference 2013	February 2013 new.emerging-research	"2013 Oral and Poster Presentation Award Winners" chers.org/2013-oral-and-poster-presentation-winners	
HONORS AND AWARDS				
	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	

WORKSHOPS

## Organizer And Presenter

2020 AFLOW School: Integrated infrastructure for computational materials discovery

Co-Organizers: Cormac Toher, David Hicks, Marco Esters, Eric Gossett, Rico Friedrich, Max J. Brenner & Stefano Curtarolo

- 8. **Presenter** at the Dresden Center for Computational Materials Science (DCMS) Materials 4.0 Summer School 2020, Technische Universität Dresden August 18, 2020.
  - "AFLOW-CHULL: Thermodynamics" recording: youtu.be/9Sa8D4inJ5w
- Presenter 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 — July 23, 2020.
  - "Materials Database and Machine Learning: AFLOW-ML" recording: youtu.be/x2qeBtOXues
- Organizer and presenter at the Texas A&M University AFLOW Multi-Day Workshop, College Station, Texas — June 16–18, 2020.
  - "Introduction to Density Functional Theory: VASP" recording: youtu.be/ChySAfo2w7g
  - "AFLOW-CHULL: Thermodynamics" recording: youtu.be/9Sa8D4inJ5w
  - "AFLOW-POCC: Disorder" recording: youtu.be/xr-mU-1ShQQ
- Presenter 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.
- Organizer and presenter at the University of Pennsylvania AFLOW Full-Day Workshop, Philadelphia, Pennsylvania — May 03, 2019.
- Organizer and presenter at the North Carolina State University AFLOW Full-Day Workshop, Raleigh, North Carolina — March 12, 2019.
- Organizer and presenter at the Carnegie Mellon University AFLOW Full-Day Workshop, Pittsburgh, Pennsylvania — January 21, 2019.
- Presenter 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.

## JOURNAL PUBLICATIONS 2020

25

Under Review

Toward Robot Science: Closed-Loop Autonomous System for Materials Exploration and Optimization (CAMEO)

**Authors**: Aaron Gilad Kusne $^{\dagger}$ , Heshan Yu $^{\dagger}$ , Changming Wu, Huairuo Zhang, Jason Hattrick-Simpers, Brian DeCost, Suchismita Sarker, Corey Oses, Cormac Toher, Stefano Curtarolo, Albert Davidov, Ritesh Agarwal, Leonid Bendersky, Mo Li, Apurva Mehta & Ichiro Takeuchi  $^{\dagger}$  contributed equally

Under Review

24 Fermi energy engineering of enhanced toughness in high entropy carbides

**Authors**: Tyler J. Harrington<sup>†</sup>, Corey Oses<sup>†</sup>, Cormac Toher, William M. Mellor, Kevin Kaufmann, Joshua Gild, Andrew Wright, Jian Luo, Stefano Curtarolo & Kenneth S. Vecchio <sup>†</sup> contributed equally

NPJ Computational Materials Discovery of novel high-entropy ceramics via machine learning

NPJ Comput. Mater. 6(42) (2020)

**Authors**: Kevin Kaufmann, Daniel Maryanovsky, William M. Mellor, Chaoyi Zhu, Alexander S. Rosengarten, Tyler J. Harrington, Corey Oses, Cormac Toher, Stefano Curtarolo & Kenneth S. Vecchio **DOI**: 10.1038/s41524-020-0317-6

Nature Reviews Materials High-entropy ceramics

Nat. Rev. Mater. 5, 295-309 (2020)

Authors: Corey Oses, Cormac Toher & Stefano Curtarolo

2019

**DOI**: 10.1038/s41578-019-0170-8

Acta Materialia

21 *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<sup>†</sup>, Tyler J. 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 Machine learning modeling of superconducting critical temperature NPJ Computational 13 NPJ Comput. Mater. 4, 29 (2018)

Materials

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<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 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 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 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

2015

Materials

Chem. Mater. **28**(18), 6484–6492 (2016)

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 Materials 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

Automated computation of materials properties

Materials Informatics: Methods, Tools and Applications, Ch. 7

Authors: Cormac Toher, Corey Oses & Stefano Curtarolo

URL: wiley.com/en-us/Materials+Informatics%3A+Methods%2C+Tools%2C+and+Applications-p-

9783527802272

2018

Machine learning and high-throughput approaches to magnetism

Book Chapter

2 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

ME 555: Computational Materials Science by Examples and

Teaching Assistant Spring 2020 Applications, Duke University Department of Mechanical

**Engineering and Materials Science** 

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

CERTIFICATIONS

Teaching Assistant

CECAM (Centre Européen de Calcul Atomique et Moléculaire)

Participant June 8–12, 2020 Open Databases Integration for Materials Design (OPTiMaDe)

Workshop at the École polytechnique fédérale de Lausanne (EPFL)

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