

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

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EDUCATION

Doctor of Philosophy	2013–2018	Duke University
	GPA: 3.8/4.0 · Department: Mechanical Engineering and Materials Science Thesis: <i>Machine learning, phase stability, and disorder with the Automatic Flow Framework for Materials Discovery</i> Advisor: Stefano Curtarolo	
Bachelor of Science	2009–2013	Cornell University
	Department: Applied and Engineering Physics Thesis: <i>Plume Propagation Simulation for Pulsed Laser Deposition</i> Advisor: Joel Brock	

PRESS AND NEWS RELEASES

MRS Bulletin	August 2017	<i>"Universal fragment descriptor predicts materials properties"</i> cambridge.org/core/journals/mrs-bulletin/news/universal-fragment-descriptor-predicts-materials-properties
UNC Eshelman School of Pharmacy	June 2017	<i>"Breakthrough Tool Predicts Properties of Theoretical Materials, Finds New Uses for Current Ones"</i> <ul style="list-style-type: none">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	<i>"Computers Create Recipe for Two New Magnetic Materials"</i> <ul style="list-style-type: none">This press release is featured on Phys.org, Slashdot, Hacker News, Reddit, engadget, The Engineer, 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	<i>"Materials fingerprints identified for informatics"</i> doi.org/10.1557/mrs.2015.76
Computational Chemistry Highlights	January 2015	<i>"Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints"</i> <ul style="list-style-type: none">"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 Research	January 2015	<i>"Molecular Tornado"</i> research.duke.edu/molecular-tornado
Duke University Graduate School	October 2014	<i>"Competing for NSF Fellowships: Advice from a Current Fellow"</i> gradschool.duke.edu/professional-development/blog/competing-nsf-fellowships-advice-current-fellow
ERN Conference 2013	February 2013	<i>"2013 Oral and Poster Presentation Award Winners"</i> new.emerging-researchers.org/2013-oral-and-poster-presentation-winners

HONORS AND AWARDS

Publication Award	2018	Editor's Choice, Publication in Comput. Mater. Sci. , Elsevier
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<i>Publication Award</i>	2017	Editor's Choice, Publication in Comput. Mater. Sci. , Elsevier
<i>Award</i>	August 14, 2015	Best Teaching Assistant Award (ME 221) , Duke University Department of Mechanical Engineering and Materials Science
<i>Publication Award</i>	2015	Editor's Choice, Publication in Comput. Mater. Sci. , Elsevier
<i>Publication Award</i>	2015	Editor's Choice, Publication in Chem. Mater. , American Chemical Society
<i>Fellowship</i>	2013–2016	Graduate Research Fellowship, National Science Foundation
<i>Award</i>	August 22, 2013	Best Presentation Award at the MEMS Departmental Retreat , Duke University Department of Mechanical Engineering and Materials Science
<i>Award</i>	March 02, 2013	First Place in Nanoscience and Physics Research Presentation , NSF / AAAS / EHR Emerging Researchers National Conference
<i>Scholarship</i>	2011–2013	Shell Incentive Fund Scholarship
<i>Scholarship</i>	2010 & 2011	Xerox Corporation Scholarship
<i>Scholarship</i>	2010 & 2011	Intel Academic Award
<i>Grant</i>	June 18, 2010	Cornell University Unmanned Air Systems Team awarded \$1,000 grant, AUVSI Student Unmanned Aerial Systems Competition
<i>Scholarship</i>	2009–2013	Meinig Family Cornell National Scholars

TALKS / PRESENTATIONS

<i>Contributed Talk</i>	2018	Universal Fragment Descriptors for Predicting Properties of Inorganic Crystals Contributed talk at the International Association for Computational Mechanics (IACM) 13 th 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.
<i>Poster Presentation</i>	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.
<i>Invited Talk</i>	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.
<i>Contributed Talk</i>	2016	Modeling Off-Stoichiometric Materials with a High-Throughput, <i>Ab-Initio</i> Approach Contributed talk at the American Physical Society March Meeting, Baltimore, Maryland — March 16, 2016.
<i>Invited Talk</i>	2016	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 2018

- Submitted* 17 *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](#)
- Journal of Chemical Information and Modeling* 16 *AFLOW-CHULL: Cloud-oriented platform for autonomous phase stability analysis*
J. Chem. Inf. Model. **in press** (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](#)
- Nature Communications* 15 *Novel high-entropy high-hardness metal carbides discovered by entropy descriptors*
Nat. Commun. **in press** (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
- MRS Bulletin* 14 *Data-driven design of inorganic materials with the Automatic Flow Framework for Materials Discovery*
MRS Bull. **43(9)**, 670–675 (2018)
Authors: [Corey Oses](#), Cormac Toher & Stefano Curtarolo
DOI: [10.1557/mrs.2018.207](#)
- NPJ Computational Materials* 13 *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* 12 *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](#)

- Acta Crystallographica Section A 11 *AFLOW-SYM: platform for the complete, automatic and self-consistent symmetry analysis of crystals*
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 10 *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 9 *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](#)
- Physical Review Materials 7 *Combining the AFLOW GIBBS and elastic Libraries to efficiently and robustly screening 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 6 *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 5 *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
- Physical Review X 4 *High-Throughput Computation of Thermal Conductivity of High-Temperature Solid 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 3 *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	2	<i>The AFLOW Standard for High-Throughput Materials Science Calculations</i> 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
Chemistry of Materials	1	<i>Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints</i> 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

2018

Submitted	3	Automated computation of materials properties Authors: Cormac Toher, Corey Oses & Stefano Curtarolo arXiv: arxiv:1805.05309
Book Chapter	2	<i>The AFLOW Fleet for Materials Discovery, Handbook of Materials Modeling. Volume 1 Methods: Theory and Modeling, in press</i> 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 arXiv: arxiv:1712.00422
Book Chapter	1	Machine learning and high-throughput approaches to magnetism, <i>Handbook of Materials Modeling. Volume 2 Applications: Current and Emerging Materials</i> Authors: Stefano Sanvito, Mario Žic, James Nelson, Thomas Archer, Corey Oses & Stefano Curtarolo DOI: 10.1007/978-3-319-50257-1_108-1

TEACHING EXPERIENCE

Teaching Assistant	Fall 2014–Spring 2015	ME 221: Structure and Properties of Solids, Duke University Department of Mechanical Engineering and Materials Science • Best Teaching Assistant Award , August 14, 2015
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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
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<i>Participant</i>	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)
<i>Graduate</i>	January 7–16, 2015	Machine Learning Summer School (MLSS) at the University of Texas at Austin
<i>Graduate</i>	May 22–27, 2011	<i>The LeaderShape Institute</i> at Cornell University
<i>Technician License</i>	July 29, 2010	American Radio Relay League (ARRL) in Roselle, New Jersey