COREY OSES

Ph.D. Candidate in Materials Science, Duke University

PERSONAL INFORMATION

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EDUCATION

2013–Present Duke University

Ph.D. Candidate GPA: 3.8/4.0 Department: Mechanical Engineering and Materials Science

Thesis: Advanced Techniques in High-Throughput Computational Materials Science

Advisor: Stefano Curtarolo

2009–2013 Cornell University

Bachelor of Science Department: Applied and Engineering Physics

Thesis: Plume Propagation Simulation for Pulsed Laser Deposition

Advisor: Joel Brock

PRESS AND NEWS RELEASES

August 2017 "Universal fragment descriptor predicts materials properties"

MRS Bulletin cambridge.org/core/journals/mrs-bulletin/news/universal-fragment-descriptor-predicts-

materials-properties

"Breakthrough Tool Predicts Properties of Theoretical Materials,

Finds New Uses for Current Ones"

UNC Eshelman School of Pharmacy

• This press release is featured on AAAS EurekAlert!, Phys.org, and ScienceDaily.

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

materials-finds-new-uses-current-ones/

Duke University Pratt School of Engineering Research April 2017 "Computers Create Recipe for Two New Magnetic Materials"

• 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

Computational Chemistry 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.

compchemhighlights.org/2015/01/materials-cartography-representing-and.html

Duke University

January 2015 "Molecular Tornado"

Research

Highlights

research.duke.edu/molecular-tornado

October 2014 "Competing for NSF Fellowships: Advice from a Current Fellow"

Duke University

gradschool.duke.edu/professional-development/blog/competing-nsf-fellowships-advice-

current-fellow

February 2013

Duke University

June 2014 "Pratt Profiles: Corey Oses"

pratt.duke.edu/graduate/diversity/pratt-profiles-corey-oses

New York Kiwanis

"New York Kiwanis Mid-Winter Conference 2013"

kiwanis-ny.org/1213/midyear.htm

New York Kiwanis

June 2012 "K-Kids Show Talent for Fundraising"

patch.com/new-york/east meadow/k-kids-show-talent-for-fundraising

New York Kiwanis

March 2012 "Past Circle K Governors Help Celebrate 50th Convention"

kiwanis-ny.org/news/view_news.php?nid=618

Cornell University

March 2011 "Undergraduate Student of the Month"

engineering.cornell.edu/diversity/about/honors/students/2011-03.cfm

HONORS AND AWARDS Publication Award 2018 Editor's Choice, Publication in Comput. Mater. Sci., Elsevier Presentation Winner at the Engineering Science Symposium, November Award 2017 SHPE National Conference Publication Award 2017 Editor's Choice, Publication in Comput. Mater. Sci., Elsevier Presentation Finalist at the Engineering Science Symposium, November Award 2016 SHPE National Conference Best Teaching Assistant Award (ME 221), Duke University Department of Mechanical Engineering and Materials Award Spring 2015 Science Editor's Choice, Publication in Comput. Mater. Sci., Elsevier Publication Award 2015 Editor's Choice, Publication in Chem. Mater., American Publication Award 2015 Chemical Society Graduate Research Fellowship, National Science Foundation Fellowship 2013-2016 Fellowship 2013-2015 Associate Fellow, National GEM Consortium Technical Poster and Paper Finalist at the Engineering November Award 2013 Science Symposium, SHPE National Conference Best Presentation Award at the MEMS Departmental Retreat, Duke University Department of Mechanical Engineering and Award August 22, 2013 Materials Science New York City Citation as Circle K Governor, Council City Citation March 21, 2013 Member Fernando Cabrera Physics First Place in Nanoscience and Presentation, NSF / AAAS / EHR Emerging Researchers Award March 2, 2013 National Conference Scholarship 2011-2013 Shell Incentive Fund Scholarship Louis Stokes Alliance for Minority Participation (LSAMP) Honor 2010-2013 Scholar Scholarship 2010 & 2011 Xerox Corporation Scholarship Scholarship 2010 & 2011 Intel Academic Award Scholarship 2010-2013 GE Foundation / LULAC Scholarship Scholarship 2009-2013 Meinig Family Cornell National Scholars Gold Medallion Winner in Engineering and Mathematics, Scholarship 2009 Hispanic Heritage Youth Awards New Jersey Principals and Supervisors Association Scholarship 2009 Scholarship Scholarship 2009 Edward J. Bloustein Distinguished Scholar Investors Savings Bank Scholarship Scholarship 2009 Superintendent's Bengal Pride Award for Excellence in Scholarship 2009 Academics and Citizenship

Scholarship 2009 Good Citizen Award, The Daughters of the American

Revolution

Honor 2008–2009 National Honor Society

TALKS / PRESENTATIONS

2018 Cloud-oriented computational phase diagrams with AFLOW-CHULL

Poster Presentation

CECAM (Centre Européen de Calcul Atomique et Moléculaire) Open Databases Integration for Materials Design (OPTiMaDe) Workshop, Lausanne, Switzerland — June 11, 2018.

2018 Universal Fragment Descriptors for Predicting Properties of Inorganic Crystals

Contributed talk at the Hopkins Extreme Materials Institute Mach Conference, Annapolis, Maryland — April 05, 2018.

Contributed Talk

Contributed talk at the SHPE National Conference, Kansas City, Missouri — November 03, 2017.

• Presentation Winner at the Engineering Science Symposium

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.

2018 Advancements in Materials Informatics with AFLOW

Invited Talk

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.

Modeling Off-Stoichiometric Materials with a High-Throughput, *Ab-Initio* Approach

Contributed Talk

Contributed talk at the SHPE National Conference, Seattle, Washington — November 04, 2016.

• Presentation Finalist at the Engineering Science Symposium

 $\textbf{Contributed talk} \ \text{at the American Physical Society March Meeting, Baltimore, Maryland} \ -- \ \text{March 16, 2016}.$

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.

Invited Talk

Contributed Talk

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.

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 SHPE National Conference, Indianapolis, Indiana — November 01, 2013.

• Technical Poster and Paper Finalist at the Engineering Science Symposium

Poster presentation at the Duke Mechanical Engineering and Materials Science (MEMS) Department Annual Retreat, Durham, North Carolina — August 22, 2013.

Best Presentation Award

3

Synchrotron Radiation Focusing Optics — Capillary Beam

Stop Design

Contributed Talk

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.

BOOK PUBLICATIONS

2018

3 Automated computation of materials properties

Submitted

Authors: Cormac Toher, Corey Oses & Stefano Curtarolo

arXiv: arxiv:1805.05309

2 Machine learning and high-throughput approaches to magnetism

Submitted

Authors: Stefano Sanvito, Mario Zic, James Nelson, Thomas Archer, Corey Oses & Stefano

Curtarolo

1 The AFLOW Fleet for Materials Discovery

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

JOURNAL PUBLICATIONS

Submitted

2018

AFLOW-CHULL: Cloud-oriented platform for autonomous phase stability analysis

Submitted

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

arXiv: arxiv:1806.06901

Autonomous data-driven materials design of inorganic compounds with

AFLOW

Submitted

Authors: Corey Oses, Cormac Toher & Stefano Curtarolo

arXiv: arxiv:1803.05035

Novel high-entropy high-hardness metal carbides discovered by entropy descriptors

Submitted

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

Machine learning modeling of superconducting critical temperature NPJ Comput. Mater. **4**(29) (2018)

NPJ Computational Materials

Authors: Valentin Stanev, Corey Oses, Aaron Gilad Kusne, Efrain Rodriguez, Johnpierre Paglione, Stefano Curtarolo & Ichiro Takeuchi

DOI: 10.1038/s41524-018-0085-8

AFLOW-ML: A RESTful API for machine-learning prediction of materials

12 properties

Computational Materials Science 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 Crystallographica Section A

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 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

AFLUX: The LUX materials search API for the AFLOW data repositories Comput. Mater. Sci. **137**, 362–370 (2017)

Computational 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

8 Crystals

7

Nat. Commun. 8, 15679 (2017)

Nature 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 thermomechanical properties of solids

Physical Review 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 Mater. **122**, 438–447 (2017)

Acta Materialia

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 Sci. Adv. **3**(4), e1602241 (2017)

Science Advances

Authors: Stefano Sanvito, Corey Oses, Junkai Xue, Anurag Tiwari, Mario Zic, 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 4 Phys. Rev. X 6(4), 041061 (2016) Physical Review X Authors: Ambroise van Roekeghem, Jesús Carrete, Corey Oses, Stefano Curtarolo & Natalio **DOI**: 10.1103/PhysRevX.6.041061 Modeling Off-Stoichiometry Materials with a High-Throughput Ab-Initio 3 Approach Chemistry of Chem. Mater. **28**(18), 6484–6492 (2016) Materials Authors: Kesong Yang, Corey Oses & Stefano Curtarolo DOI: 10.1021/acs.chemmater.6b01449 2015 The AFLOW Standard for High-Throughput Materials Science Calculations 2 Comput. Mater. Sci. 108A, 233-238 (2015) Computational Authors: Camilo E. Calderon, Jose J. Plata, Cormac Toher, Corey Oses, Ohad Levy, Marco Fornari, Materials Science 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 1 Chem. Mater. 27(3), 735–743 (2015) Chemistry of Authors: Olexandr Isayev, Denis Fourches, Eugene N. Muratov, Corey Oses, Kevin M. Rasch, Materials Alexander Tropsha & Stefano Curtarolo • This paper was selected for Editor's Choice. DOI: 10.1021/cm503507h TEACHING EXPERIENCE ME 221: Structure and Properties of Solids, Duke University Fall 2014-Spring Department of Mechanical Engineering and Materials Teaching Assistant 2015 Science • Best Teaching Assistant Award, Spring 2015 WORK EXPERIENCE Cornell High Energy Synchrotron Source (BioSAXS on F2 Summer 2013 and G Beamlines) Internship Supervisors: Richard Edward Gillilan & Ernest Fontes Summer 2012 Cornell High Energy Synchrotron Source Internship Supervisors: Rong Huang & Ernest Fontes CERTIFICATIONS Machine Learning Summer School (MLSS) at Duke Graduate June 25-29, 2018 University CECAM (Centre Européen de Calcul Atomique et Moléculaire) Open Databases Integration for Materials Participant June 11-15, 2018 Design (OPTiMaDe) Workshop at the École polytechnique fédérale de Lausanne (EPFL) September 26-29, Graduate NextProf Workshop at the University of Michigan 2017 Machine Learning Summer School (MLSS) at the University 7–16, January Graduate 2015 of Texas at Austin

The Leader Shape Institute at Cornell University

Graduate

May 22-27, 2011

Technician License	July 29, 2010	American Radio Relay League (ARRL) in Roselle, New Jersey
ACTIVITIES AND OUTREACH		
Graduate Representative	2015–Present	Council of Presidents, Duke University Graduate School
Member	2014–Present	American Physical Society
Graduate Student Advisor	2009–Present	Society of Hispanic Professional Engineers, Duke University & Cornell University
	Positions: Graduat	e Student Advisor, President, Corporate Vice President & Treasurer
Undergraduate Researcher	2011–2013	Brock Research Group, Cornell University
Distinguished Past Governor	2010–2013	Circle K, Cornell University
	Positions : New York District Distinguished Past Governor, New York District Distinguished Past Treasurer & Restarting Chapter President at Cornell University	
Mechanical Engineer	2009–2011	Cornell University Autonomous Flight Team, Cornell University
	Positions: Mechanical Engineer, Safety Officer & Systems Manager	