COREY OSES

Ph.D. Candidate in Materials Science, Duke University

PERSONAL INFORMATION

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

website coreyoses.com

EDUCATION

Ph.D. Candidate 2013–Present Duke University

GPA: 3.8/4.0 · Department: Mechanical Engineering and Materials Science Thesis: Advanced Techniques in High-Throughput Computational Materials Science

Advisor: Stefano Curtarolo

Bachelor of Science 2009–2013 Cornell University

Department: Applied and Engineering Physics

Thesis: Plume Propagation Simulation for Pulsed Laser Deposition

Advisor: Joel Brock

PRESS AND NEWS RELEASES

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

cambridge.org/core/journals/mrs-bullet in/news/universal-fragment-descriptor-predicts-materials-product of the control of th

properties

UNC Eshelman June 2017 "Breakthrough Tool Predicts Properties of Theoretical Materials, Finds

School of Pharmacy

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/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/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/breakthrough-tool-pharmacy.unc.edu/news/2017/06/breakthrough-tool-pharmacy.unc.edu/news/2017/06/breakthrough-tool-pharmacy.unc.edu/news/2017/06/breakthrough-tool-pharmacy.unc.edu/news/2017/06/breakthrough-tool-pharmacy.unc.edu/news/2017/06/breakthrough-tool-pharmacy.unc.edu/news/2017/06/breakthrough-tool-pharmacy.unc.edu/news/2017/06/breakthrough-tool-pharmacy.unc.edu/news/2017/06/breakthrough-tool-pharmacy.unc.edu/news/2017/06/breakthrough-tool-pharmacy.unc.edu/news/2017/06/breakthrough-tool-pharmacy.unc.edu/news/2017/06/breakthrough-tool-pharmacy.unc.edu/news/2017/06/breakthrough-tool-pharmacy.unc.edu/ne

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, The Engineer, Science Alert, Azo Materials, Next Big Future, Futurism, New Atlas, and International Business Times.

pratt.duke.edu/about/news/predicting-magnets

Computational January 2015 "Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints"

. Chemistry Highlights

 "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 research.duke.edu/molecular-tornado

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

Graduate School gradschool.duke.edu/professional-development/blog/competing-nsf-fellowships-advice-current-fellow

Duke University June 2014 "Pratt Profiles: Corey Oses" Pratt School of pratt.duke.edu/graduate/diversity/pratt-profiles-corey-oses

Engineering

Duke University November 2013 "Society of Hispanic Professional Engineers"

MEM Program memp.pratt.duke.edu/news/society-hispanic-professional-engineers

New York Kiwanis February 2013 "New York Kiwanis Mid-Winter Conference 2013"

kiwanis-ny.org/1213/midyear.htm

ERN Conference February 2013 "2013 Oral and Poster Presentation Award Winners"

2013 new.emerging-researchers.org/2013-oral-and-poster-presentation-winners

New York Kiwanis June 2012 "K-Kids Show Talent for Fundraising"

patch.com/new-york/eastmeadow/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

HONORS AND AWARDS

Publication Award	2018	Editor's Choice, Publication in Comput. Mater. Sci., Elsevier
Award	November 3, 2017	Presentation Winner at the Engineering Science Symposium, SHPE National Conference
Publication Award	2017	Editor's Choice, Publication in Comput. Mater. Sci., Elsevier
Award	November 4, 2016	Presentation Finalist at the Engineering Science Symposium, SHPE National Conference
Award	Spring 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
Fellowship	2013–2015	Associate Fellow, National GEM Consortium
Award	November 1, 2013	Technical Poster and Paper Finalist at the Engineering Science Symposium, SHPE National Conference
Award	August 22, 2013	Best Presentation Award at the MEMS Departmental Retreat, Duke University Department of Mechanical Engineering and Materials Science
City Citation	March 21, 2013	New York City Citation as Circle K Governor, Council Member Fernando Cabrera
Award	March 2, 2013	First Place in Nanoscience and Physics Research Presentation, NSF / AAAS / EHR Emerging Researchers National Conference
Award	October 8, 2011	College Bowl Winner, Hispanic Engineer National Achievement Awards Conference (HENAAC)
Scholarship	2011–2013	Shell Incentive Fund Scholarship
Honor	2010–2013	Louis Stokes Alliance for Minority Participation (LSAMP) 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
Scholarship	2009	Gold Medallion Winner in Engineering and Mathematics, Hispanic Heritage Youth Awards
Scholarship	2009	New Jersey Principals and Supervisors Association Scholarship
Scholarship	2009	Edward J. Bloustein Distinguished Scholar
Scholarship	2009	Investors Savings Bank Scholarship
Scholarship	2009	Superintendent's Bengal Pride Award for Excellence in Academics and Citizenship
Scholarship	2009	Good Citizen Award, The Daughters of the American Revolution

Honor 2008–2009 National Honor Society

TALKS / PRESENTATIONS

Poster Presentation 2018 Clurify 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.

Contributed Talk 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 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

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 2016 Modeling Off-Stoichiometric Materials with a High-Throughput, Ab-Initio Approach

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

• Presentation Finalist at the Engineering Science Symposium

Contributed talk at the American Physical Society March Meeting, Baltimore, Maryland — March 16, 2016.

Invited Talk 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 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

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.

BOOK PUBLICATIONS

2018

2018

Submitted 3 Automated computation of materials properties

Authors: Cormac Toher, Corey Oses & Stefano Curtarolo

arXiv: arxiv:1805.05309

Submitted 2 Machine learning and high-throughput approaches to magnetism

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

Submitted 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 16 AFLOW-CHULL: Cloud-oriented platform for autonomous phase stability analysis

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

Submitted 15 Autonomous data-driven materials design of inorganic compounds with AFLOW

Authors: Corey Oses, Cormac Toher & Stefano Curtarolo

arXiv: arxiv:1803.05035

Submitted 14 Novel high-entropy high-hardness metal carbides discovered by entropy descriptors

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

† contributed equally

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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

11 analysis of crystals

Crystallographica

Acta

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 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 *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 *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 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

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

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

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

TEACHING EXPERIENCE

Fall 2014–Spring ME 221: Structure and Properties of Solids, Duke University Teaching Assistant Department of Mechanical Engineering and Materials Science 2015

• Best Teaching Assistant Award, Spring 2015

WORK EXPERIENCE

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

CERTIFICATIONS

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)

September 26-29, Graduate

2017

NextProf Workshop at the University of Michigan

January 7–16, Graduate

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

ACTIVITIES AND OUTREACH

2015-Present Graduate

Council of Presidents, Duke University Graduate School

Representative

American Physical Society Member 2014-Present

Society of Hispanic Professional Engineers, Duke University & Graduate Student 2009-Present

Cornell University

Advisor

Positions: Graduate Student Advisor, President, Corporate Vice President & Treasurer

Brock Research Group, Cornell University Undergraduate 2011-2013

Researcher

Distinguished Past 2010-2013 Circle K, Cornell University

> Governor Positions: New York District Distinguished Past Governor, New York District Distinguished Past Treasurer

> > & Restarting Chapter President at Cornell University

Mechanical 2009-2011 Cornell University Autonomous Flight Team, Cornell University

Engineer Positions: Mechanical Engineer, Safety Officer & Systems Manager