COREY OSES

Ph.D. Candidate in Materials Science, Duke University

PERSONAL INFORMATION

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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-bulletin/news/universal-fragment-descriptor-predicts-materials-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-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 Highlights

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 Research

January 2015 *"Molecular Tornado"*

research.duke.edu/molecular-tornado

Duke University

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

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

Duke University

June 2014 *"Pratt Profiles: Corey Oses"*

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

Duke University Master of Engineering Management

November 2013 *"Society of Hispanic Professional Engineers"*

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

Emerging Researchers National Conference	*February 2013*	*"2013 Oral and Poster Presentation Award Winners"* 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
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
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
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*

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.

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.

2015 Plume Propagation Simulation for Pulsed Laser Deposition

Contributed Talk

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

2013 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

Submitted

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

2018

16 *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

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

Submitted

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

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 Zic, 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 *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

Chemistry of Materials

1 *Materials Cartography: Representing and Mining Materials Space Using Structural 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

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, Spring 2015

Work Experience

Internship — *Summer 2013* — Cornell High Energy Synchrotron Source (BioSAXS on F2 and G Beamlines)

Supervisors: Richard Edward Gillilan & Ernest Fontes

Internship — *Summer 2012* — Cornell High Energy Synchrotron Source

Supervisors: Rong Huang & Ernest Fontes

Certifications

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	*September 26–29, 2017*	*NextProf* Workshop at the University of Michigan
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

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: Graduate 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	