COREY OSES

Ph.D. Candidate in Materials Science, Duke University

PERSONAL INFORMATION

email	corey.oses@duke.edu
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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 — *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 Graduate School — *October 2014* — *"Competing for NSF Fellowships: Advice from a Current Fellow"*
gradschool.duke.edu/professional-development/blog/competing-nsf-fellowships-advice-current-fellow

ERN Conference 2013 — *February 2013* — *"2013 Oral and Poster Presentation Award Winners"*
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
Publication Award	*2017*	Editor's Choice, Publication in Comput. Mater. Sci., Elsevier
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
Award	*August 22, 2013*	Best Presentation Award at the MEMS Departmental Retreat, Duke University Department of Mechanical Engineering and Materials Science
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
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

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 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 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 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

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

2018

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

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 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

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