

COREY OSES

Ph.D. Candidate in Materials Science, Duke University

PERSONAL INFORMATION

email corey.oses@duke.edu
phone (M) +1 (201) 674 1407 · (W) +1 (919) 684 1553
website coreyoses.com

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

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!](http://AAASEurekAlert!) and Phys.org.
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

New York Kiwanis February 2013 “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/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

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| Publication Award | 2018 | | Editor’s Choice, Publication in Comput. Mater. Sci. , Elsevier |
| Award | November 2017 | 3, | Presentation Winner at the Engineering Science Symposium , SHPE National Conference |
| Publication Award | 2017 | | Editor’s Choice, Publication in Comput. Mater. Sci. , Elsevier |
| Award | November 2016 | 4, | 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 2013 | 1, | 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 |

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| <i>Scholarship</i> | 2009 | Good Citizen Award, The Daughters of the American Revolution |
| <i>Honor</i> | 2008–2009 | National Honor Society |

TALKS / PRESENTATIONS

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| <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>Contributed Talk</i> | 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. |
| <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 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. |
| <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. |
| <i>Contributed Talk</i> | 2014 | Plume Propagation Simulation for Pulsed Laser Deposition 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. Contributed Talk 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

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| 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. Chepulsii, 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

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| Submitted | 16 <i>AFLOW-CHULL: Cloud-oriented platform for autonomous phase stability analysis</i> 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 <i>Autonomous data-driven materials design of inorganic compounds with AFLOW</i> Authors: Corey Oses , Cormac Toher & Stefano Curtarolo arXiv: arxiv:1803.05035 |
| Submitted | 14 <i>Novel high-entropy high-hardness metal carbides discovered by entropy descriptors</i> 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 <i>Machine learning modeling of superconducting critical temperature</i> 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 |

- 2017
- 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](#)
- 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. Coe & Stefano Curtarolo
DOI: [10.1126/sciadv.1602241](#)
- 2016

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| Physical Review X | 4 | <i>High-Throughput Computation of Thermal Conductivity of High-Temperature Solid Phases: The Case of Oxide and Fluoride Perovskites</i> 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 | <i>Modeling Off-Stoichiometry Materials with a High-Throughput Ab-Initio Approach</i> 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 |

TEACHING EXPERIENCE

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|--------------------|-----------------------|---|
| 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

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|------------|-------------|--|
| 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

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|-------------|-----------------------|--|
| 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 29–29, 2010* American Radio Relay League (ARRL) in Roselle, New Jersey

ACTIVITIES AND OUTREACH

| | | |
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| <i>Graduate Representative</i> | <i>2015–Present</i> | Council of Presidents, Duke University Graduate School |
| <i>Member</i> | <i>2014–Present</i> | American Physical Society |
| <i>Graduate Student Advisor</i> | <i>2009–Present</i> | Society of Hispanic Professional Engineers, Duke University & Cornell University Positions: Graduate Student Advisor, President , Corporate Vice President & Treasurer |
| <i>Undergraduate Researcher</i> | <i>2011–2013</i> | Brock Research Group, Cornell University |
| <i>Distinguished Past Governor</i> | <i>2010–2013</i> | Circle K, Cornell University Positions: New York District Distinguished Past Governor , New York District Distinguished Past Treasurer & Restarting Chapter President at Cornell University |
| <i>Mechanical Engineer</i> | <i>2009–2011</i> | Cornell University Autonomous Flight Team, Cornell University Positions: Mechanical Engineer, Safety Officer & Systems Manager |