

# COREY OSES

Ph.D. Candidate in Materials Science, Duke University

## PERSONAL INFORMATION

email	<a href="mailto:corey.oses@duke.edu">corey.oses@duke.edu</a>
phone	(W) +1 (919) 684 1553
website	<a href="http://coreyoses.com">coreyoses.com</a>

## EDUCATION

Ph.D. Candidate	2013–Present	Duke University
	GPA: 3.8/4.0 · Department: Mechanical Engineering and Materials Science Thesis: <i>Advanced Techniques in High-Throughput Computational Materials Science</i> <b>Advisor:</b> Stefano Curtarolo	
Bachelor of Science	2009–2013	Cornell University
	Department: Applied and Engineering Physics Thesis: <i>Plume Propagation Simulation for Pulsed Laser Deposition</i> <b>Advisor:</b> Joel Brock	

## PRESS AND NEWS RELEASES

MRS Bulletin	August 2017	<i>“Universal fragment descriptor predicts materials properties”</i> <a href="http://cambridge.org/core/journals/mrs-bulletin/news/universal-fragment-descriptor-predicts-materials-properties">cambridge.org/core/journals/mrs-bulletin/news/universal-fragment-descriptor-predicts-materials-properties</a>
UNC Eshelman School of Pharmacy	June 2017	<i>“Breakthrough Tool Predicts Properties of Theoretical Materials, Finds New Uses for Current Ones”</i> <ul style="list-style-type: none"><li>This press release is featured on <a href="#">AAAS EurekAlert!</a>, <a href="#">Phys.org</a>, and <a href="#">ScienceDaily</a>. <a href="http://pharmacy.unc.edu/news/2017/06/06/breakthrough-tool-predicts-properties-theoretical-materials-finds-new-uses-current-ones/">pharmacy.unc.edu/news/2017/06/06/breakthrough-tool-predicts-properties-theoretical-materials-finds-new-uses-current-ones/</a></li></ul>
Duke University Pratt School of Engineering	April 2017	<i>“Computers Create Recipe for Two New Magnetic Materials”</i> <ul style="list-style-type: none"><li>This press release is featured on <a href="#">Phys.org</a>, <a href="#">Slashdot</a>, <a href="#">Hacker News</a>, <a href="#">Reddit</a>, <a href="#">engadget</a>, <a href="#">The Engineer</a>, <a href="#">Science Alert</a>, <a href="#">Azo Materials</a>, <a href="#">Next Big Future</a>, <a href="#">Futurism</a>, <a href="#">New Atlas</a>, and <a href="#">International Business Times</a>. <a href="http://pratt.duke.edu/about/news/predicting-magnets">pratt.duke.edu/about/news/predicting-magnets</a></li></ul>
Computational Chemistry Highlights	January 2015	<i>“Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints”</i> <ul style="list-style-type: none"><li>“This paper is a <i>tour de force</i> for computational materials science” — Prof. Alán Aspuru-Guzik, Harvard University. <a href="http://compchemhighlights.org/2015/01/materials-cartography-representing-and.html">compchemhighlights.org/2015/01/materials-cartography-representing-and.html</a></li></ul>
Duke University Research	January 2015	<i>“Molecular Tornado”</i> <a href="http://research.duke.edu/molecular-tornado">research.duke.edu/molecular-tornado</a>
Duke University Graduate School	October 2014	<i>“Competing for NSF Fellowships: Advice from a Current Fellow”</i> <a href="http://gradschool.duke.edu/professional-development/blog/competing-nsf-fellowships-advice-current-fellow">gradschool.duke.edu/professional-development/blog/competing-nsf-fellowships-advice-current-fellow</a>
ERN Conference 2013	February 2013	<i>“2013 Oral and Poster Presentation Award Winners”</i> <a href="http://new.emerging-researchers.org/2013-oral-and-poster-presentation-winners">new.emerging-researchers.org/2013-oral-and-poster-presentation-winners</a>

## HONORS AND AWARDS

Publication Award	2018	Editor’s Choice, <a href="#">Publication in Comput. Mater. Sci.</a> , Elsevier
Publication Award	2017	Editor’s Choice, <a href="#">Publication in Comput. Mater. Sci.</a> , Elsevier
Award	August 14, 2015	<a href="#">Best Teaching Assistant Award (ME 221)</a> , Duke University Department of Mechanical Engineering and Materials Science
Publication Award	2015	Editor’s Choice, <a href="#">Publication in Comput. Mater. Sci.</a> , Elsevier

<i>Publication Award</i>	2015	Editor's Choice, <b>Publication in Chem. Mater.</b> , American Chemical Society
<i>Fellowship</i>	2013–2016	Graduate Research Fellowship, National Science Foundation
<i>Award</i>	August 22, 2013	<b>Best Presentation Award at the MEMS Departmental Retreat</b> , Duke University Department of Mechanical Engineering and Materials Science
<i>Award</i>	March 02, 2013	<b>First Place in Nanoscience and Physics Research Presentation</b> , NSF / AAAS / EHR Emerging Researchers National Conference
<i>Scholarship</i>	2011–2013	Shell Incentive Fund Scholarship
<i>Scholarship</i>	2010 & 2011	Xerox Corporation Scholarship
<i>Scholarship</i>	2010 & 2011	Intel Academic Award
<i>Grant</i>	June 18, 2010	Cornell University Unmanned Air Systems Team awarded \$1,000 grant, AUVSI Student Unmanned Aerial Systems Competition
<i>Scholarship</i>	2009–2013	Meinig Family Cornell National Scholars

## TALKS / PRESENTATIONS

<i>Contributed Talk</i>	2018	<p>Universal Fragment Descriptors for Predicting Properties of Inorganic Crystals</p> <p><b>Contributed talk</b> at the International Association for Computational Mechanics (IACM) 13<sup>th</sup> World Congress in Computational Mechanics (WCCM), New York City, New York — July 23, 2018.</p> <p><b>Contributed talk</b> at the Hopkins Extreme Materials Institute Mach Conference, Annapolis, Maryland — April 05, 2018.</p> <p><b>Contributed talk</b> at the Duke University Chemistry Department Third Annual Graduate Research Symposium, Durham, North Carolina — October 09, 2017.</p> <p><b>Contributed talk</b> at the American Physical Society March Meeting, New Orleans, Louisiana — March 14, 2017.</p>
<i>Poster Presentation</i>	2018	<p>Cloud-oriented computational phase diagrams with AFLOW-CHULL</p> <p>CECAM (Centre Européen de Calcul Atomique et Moléculaire) Open Databases Integration for Materials Design (OPTiMaDe) Workshop, Lausanne, Switzerland — June 11, 2018.</p>
<i>Invited Talk</i>	2018	<p>Advancements in Materials Informatics with AFLOW</p> <p><b>Invited talk</b> at the Fritz-Haber-Institut der Max-Planck-Gesellschaft Theory Department Seminar, Berlin, Germany — January 18, 2018.</p> <p><b>Invited talk</b> at the Humboldt University of Berlin Physics Department Seminar, Berlin, Germany — January 16, 2018.</p>
<i>Contributed Talk</i>	2016	<p>Modeling Off-Stoichiometric Materials with a High-Throughput, <i>Ab-Initio</i> Approach</p> <p><b>Contributed talk</b> at the American Physical Society March Meeting, Baltimore, Maryland — March 16, 2016.</p>
<i>Invited Talk</i>	2016	<p>Materials Cartography: Representing and Mining Materials Space using Structural and Electronic Fingerprints</p> <p><b>Invited talk</b> at the Brigham Young University Condensed Matter Physics Seminar, Provo, Utah — February 18, 2016.</p> <p><b>Contributed talk</b> at the Duke Mechanical Engineering and Materials Science (MEMS) Department Graduate Student Seminar, Durham, North Carolina — September 25, 2015.</p> <p><b>Contributed talk</b> at the American Physical Society March Meeting, San Antonio, Texas — March 02, 2015.</p>
<i>Contributed Talk</i>	2015	<p>Plume Propagation Simulation for Pulsed Laser Deposition</p> <p><b>Poster presentation</b> at the University of Texas at Austin Machine Learning Summer School (MLSS), Austin, Texas — January 12, 2015.</p> <p><b>Contributed talk</b> at the NSF / AAAS / EHR Emerging Researchers National Conference, Washington, D.C. — February 22, 2014.</p> <p><b>Poster presentation</b> at the MRS / ASM / AVS / AREMS Meeting, North Carolina State University, Raleigh, North Carolina — November 15, 2013.</p> <p><b>Poster presentation</b> at the Duke Mechanical Engineering and Materials Science (MEMS) Department Annual Retreat, Durham, North Carolina — August 22, 2013.</p> <ul style="list-style-type: none"> <li>• <a href="#">Best Presentation Award</a></li> </ul>

- 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.

## JOURNAL PUBLICATIONS

2018

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| Submitted                                    | 17 | <i>AFLOW-QHA3P: Robust and automated method to compute thermodynamic properties of solids</i><br><b>Authors:</b> Pinku Nath, Demet Usanmaz, David Hicks, <a href="#">Corey Oses</a> , Marco Fornari, Marco Buongiorno Nardelli, Cormac Toher & Stefano Curtarolo<br><b>arXiv:</b> <a href="#">arxiv:1807.04669</a>   |
| Submitted                                    | 16 | <i>Novel high-entropy high-hardness metal carbides discovered by entropy descriptors</i><br><b>Authors:</b> Pranab Sarker <sup>†</sup> , Tyler Harrington <sup>†</sup> , Cormac Toher, <a href="#">Corey Oses</a> , Mojtaba Samiee, Jon-Paul Maria, Donald W. Brenner, Kenneth S. Vecchio & Stefano Curtarolo<br><sup>†</sup> contributed equally  |
| Journal of Chemical Information and Modeling | 15 | <i>AFLOW-CHULL: Cloud-oriented platform for autonomous phase stability analysis</i><br><b>J. Chem. Inf. Model. in press</b> (2018)<br><b>Authors:</b> <a href="#">Corey Oses</a> , 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<br><b>DOI:</b> <a href="#">10.1021/acs.jcim.8b00393</a>  |
| MRS Bulletin                                 | 14 | <i>Data-driven design of inorganic materials with the Automatic Flow Framework for Materials Discovery</i><br><b>MRS Bull. 43(9), 670–675</b> (2018)<br><b>Authors:</b> <a href="#">Corey Oses</a> , Cormac Toher & Stefano Curtarolo<br><b>DOI:</b> <a href="#">10.1557/mrs.2018.207</a>  |
| NPJ Computational Materials                  | 13 | <i>Machine learning modeling of superconducting critical temperature</i><br><b>NPJ Comput. Mater. 4(29)</b> (2018)<br><b>Authors:</b> Valentin Stanev, <a href="#">Corey Oses</a> , Aaron Gilad Kusne, Efrain Rodriguez, Johnpierre Paglione, Stefano Curtarolo & Ichiro Takeuchi<br><b>DOI:</b> <a href="#">10.1038/s41524-018-0085-8</a>   |
| Computational Materials Science              | 12 | <i>AFLOW-ML: A RESTful API for machine-learning prediction of materials properties</i><br><b>Comput. Mater. Sci. 152, 134–145</b> (2018)<br><b>Authors:</b> Eric Gossett, Cormac Toher, <a href="#">Corey Oses</a> , Olexandr Isayev, Fleur Legrain, Frisco Rose, Eva Zurek, Jesús Carrete, Natalio Mingo, Alexander Tropsha & Stefano Curtarolo<br>• This paper was selected for <a href="#">Editor's Choice</a> .<br><b>DOI:</b> <a href="#">10.1016/j.commatsci.2018.03.075</a> |
| Acta Crystallographica Section A             | 11 | <i>AFLOW-SYM: platform for the complete, automatic and self-consistent symmetry analysis of crystals</i><br><b>Acta Cryst. A 74, 184–203</b> (2018)<br><b>Authors:</b> David Hicks, <a href="#">Corey Oses</a> , Eric Gossett, Geena Gomez, Richard H. Taylor, Cormac Toher, Michael J. Mehl, Ohad Levy & Stefano Curtarolo<br><b>DOI:</b> <a href="#">10.1107/S2053273318003066</a>   |

2017

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| Inorganic Chemistry | 10 | <i>The structure and composition statistics of 6A binary and ternary structures</i><br><b>Inorg. Chem. 57(2), 653–667</b> (2017)<br><b>Authors:</b> Alon Hever, <a href="#">Corey Oses</a> , Stefano Curtarolo, Ohad Levy & Amir Natan<br><b>DOI:</b> <a href="#">10.1021/acs.inorgchem.7b02462</a> |
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- 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<sup>†</sup>, [Corey Oses](#)<sup>†</sup>, Cormac Toher, Eric Gossett, Stefano Curtarolo & Alexander Tropsha  
<sup>†</sup> 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](#)

## BOOK PUBLICATIONS

### 2018

<i>Submitted</i>	3	Automated computation of materials properties <b>Authors:</b> Cormac Toher, <a href="#">Corey Oses</a> & Stefano Curtarolo <b>arXiv:</b> <a href="#">arxiv:1805.05309</a>
<i>Submitted</i>	2	Machine learning and high-throughput approaches to magnetism <b>Authors:</b> Stefano Sanvito, Mario Zic, James Nelson, Thomas Archer, <a href="#">Corey Oses</a> & Stefano Curtarolo
<i>Book Chapter</i>	1	The AFLOW Fleet for Materials Discovery, <i>Handbook of Materials Modeling. Volume 1 Methods: Theory and Modeling</i> , <b>in press</b> <b>Authors:</b> Cormac Toher, <a href="#">Corey Oses</a> , 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 <b>arXiv:</b> <a href="#">arxiv:1712.00422</a>

## TEACHING EXPERIENCE

<i>Teaching Assistant</i>	Fall 2014–Spring 2015	ME 221: Structure and Properties of Solids, Duke University Department of Mechanical Engineering and Materials Science • <a href="#">Best Teaching Assistant Award</a> , August 14, 2015
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## WORK EXPERIENCE

<i>Internship</i>	Summer 2013	Cornell High Energy Synchrotron Source (BioSAXS on F2 and G Beamlines) <b>Supervisors:</b> Richard E. Gillilan & Ernest Fontes
<i>Internship</i>	Summer 2012	Cornell High Energy Synchrotron Source (Capillary Optics Group) <b>Supervisors:</b> Rong Huang & Ernest Fontes
<i>Office Assistant</i>	Summer 2011	ILR Budget Office, Cornell University <b>Supervisor:</b> Renee Monroe Cook

## CERTIFICATIONS

<i>Graduate</i>	June 25–29, 2018	Machine Learning Summer School (MLSS) at Duke University
<i>Participant</i>	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)
<i>Graduate</i>	January 7–16, 2015	Machine Learning Summer School (MLSS) at the University of Texas at Austin
<i>Graduate</i>	May 22–27, 2011	<i>The LeaderShape Institute</i> at Cornell University
<i>Technician License</i>	July 29, 2010	American Radio Relay League (ARRL) in Roselle, New Jersey