# COREY OSES

*Materials Science*, Duke University



## PERSONAL INFORMATION


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|---|---|
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| phone | (W) +1 (919) 684 1553 |
| website | coreyoses.com |


## WORK EXPERIENCE

*Postdoctoral Fellow* — 2018–present — Duke University

**Supervisor**: Stefano Curtarolo

*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

## EDUCATION

*Ph.D.* — 2013–2018 — Duke University

**GPA**: 3.8/4.0 · **Department**: Mechanical Engineering and Materials Science
**Thesis**: *Machine learning, phase stability, and disorder with the Automatic Flow Framework for Materials Discovery*
**ProQuest**: search.proquest.com/docview/2172402640?pq-origsite=gscholar
**Advisor**: Stefano Curtarolo

*B.Sc.* — 2009–2013 — Cornell University

**Department**: Applied and Engineering Physics
**Thesis**: *Plume Propagation Simulation for Pulsed Laser Deposition*
**Advisor**: Joel Brock

## PRESS AND NEWS RELEASES

*Duke University Pratt School of Engineering* — November 2018 — *"Disordered Materials Could Be Hardest, Most Heat-Tolerant Ever"*

- This press release is featured on AAAS EurekAlert!, Phys.org, ScienceDaily, Science Bulletin, Naaju, NewsBeezer, RemoNews, Tech2, and LongRoom News.

pratt.duke.edu/about/news/chaotic-carbides

*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, Engineering.com, Science Alert, Azo Materials, Next Big Future, Futurism, New Atlas, and International Business Times.

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

*MRS Bulletin* — April 2015 — *"Materials fingerprints identified for informatics"*

doi.org/10.1557/mrs.2015.76

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| *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

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|---|---|---|
| *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

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|---|---|---|
| *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* | August 14, 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 02, 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

*Invited Seminar* 2019 AFLOW: Integrated infrastructure for computational materials discovery

**Co-Presenters**: Cormac Toher, David Hicks, Marco Esters, Eric Gossett, Max J. Brenner & Stefano Curtarolo
**Invited seminar** at the NIST/Moore Foundation/University of Maryland Machine Learning for Materials Research Bootcamp 2019 & Workshop on Machine Learning Quantum Materials, Institute for Bioscience & Biotechnology Research in Gaithersburg, Maryland — August 05, 2019.
**Invited seminar** at the University of Pennsylvania AFLOW Full-Day Workshop, Philadelphia, Pennsylvania — May 03, 2019.
**Invited seminar** at the North Carolina State University AFLOW Full-Day Workshop, Raleigh, North Carolina — March 12, 2019.
**Invited seminar** at the Carnegie Mellon University AFLOW Full-Day Workshop, Pittsburgh, Pennsylvania — January 21, 2019.
**Invited seminar** at the NIST/Moore Foundation/University of Maryland Machine Learning for Materials Research Bootcamp 2018 & Workshop on Machine Learning Quantum Materials, Institute for Bioscience & Biotechnology Research in Gaithersburg, Maryland — August 02, 2018.

*Contributed Talk* 2019 Cloud-oriented computational phase diagrams with AFLOW-CHULL

**Contributed talk** at the American Physical Society March Meeting, Boston, Massachusetts — March 07, 2019.
**Poster presentation** at the CECAM (Centre Européen de Calcul Atomique et Moléculaire) Open Databases Integration for Materials Design (OPTiMaDe) Workshop, Lausanne, Switzerland — June 11, 2018.

*Invited Talk* 2019 Going Off-Stoichiometry: Challenging Traditional Materials Discovery

Naval Research Laboratory Center for Computational Materials Science Seminar, Washington, D.C. — January 09, 2019.

*Contributed Talk* 2018 Universal Fragment Descriptors for Predicting Properties of Inorganic Crystals

**Contributed talk** at the International Association for Computational Mechanics (IACM) 13th World Congress in Computational Mechanics (WCCM), New York City, New York — July 23, 2018.
**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.

## JOURNAL PUBLICATIONS

### 2019

*Under Review* 23 *Discovery of novel high-entropy ceramics via machine learning*

**Authors**: Kevin Kaufmann, Daniel Maryanovsky, William M. Mellor, Chaoyi Zhu, Alexander S. Rosengarten, Tyler J. Harrington, Corey Oses, Cormac Toher, Stefano Curtarolo & Kenneth S. Vecchio

*Nature Reviews Materials*

22 *High-entropy ceramics*
Nat. Rev. Mater. **in press** (2019)
**Authors**: Corey Oses, Cormac Toher & Stefano Curtarolo

*Acta Materialia*

21 *Metallic glasses for biodegradable implants*
Acta Mater. **176**, 297–305 (2019)
**Authors**: Denise C. Ford, David Hicks, Corey Oses, Cormac Toher & Stefano Curtarolo
**DOI**: 10.1016/j.actamat.2019.07.008

*NPJ Computational Materials*

20 *Predicting Superhard Materials via a Machine Learning Informed Evolutionary Structure Search*
NPJ Comput. Mater. **5**, 89 (2019)
**Authors**: Patrick Avery, Xiaoyu Wang, Corey Oses, Eric Gossett, Davide M. Proserpio, Cormac Toher, Stefano Curtarolo & Eva Zurek
**DOI**: 10.1038/s41524-019-0226-8

*NPJ Computational Materials*

19 *Unavoidable disorder and entropy in multi-component systems*
NPJ Comput. Mater. **5**, 69 (2019)
**Authors**: Cormac Toher, Corey Oses, David Hicks & Stefano Curtarolo
**DOI**: 10.1038/s41524-019-0206-z

*NPJ Computational Materials*

18 *Coordination corrected ab initio formation enthalpies*
NPJ Comput. Mater. **5**, 59 (2019)
**Authors**: Rico Friedrich, Demet Usanmaz, Corey Oses, Andrew R. Supka, Marco Fornari, Marco Buongiorno Nardelli, Cormac Toher & Stefano Curtarolo
**DOI**: 10.1038/s41524-019-0192-1

*Physical Review Materials*

17 *AFLOW-QHA3P: Robust and automated method to compute thermodynamic properties of solids*
Phys. Rev. Mater. **3**, 073801 (2019)
**Authors**: Pinku Nath, Demet Usanmaz, David Hicks, Corey Oses, Marco Fornari, Marco Buongiorno Nardelli, Cormac Toher & Stefano Curtarolo
**DOI**: 10.1103/PhysRevMaterials.3.073801

## 2018

*Journal of Chemical Information and Modeling*

16 *AFLOW-CHULL: Cloud-oriented platform for autonomous phase stability analysis*
J. Chem. Inf. Model. **58**(12), 2477–2490 (2018)
**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
**DOI**: 10.1021/acs.jcim.8b00393

*MRS Bulletin*

15 *Data-driven design of inorganic materials with the Automatic Flow Framework for Materials Discovery*
MRS Bull. **43**(9), 670–675 (2018)
**Authors**: Corey Oses, Cormac Toher & Stefano Curtarolo
**DOI**: 10.1557/mrs.2018.207

*Nature Communications*

14 *Novel high-entropy high-hardness metal carbides discovered by entropy descriptors*
Nat. Commun. **9**, 4980 (2018)
**Authors**: Pranab Sarker†, Tyler J. Harrington†, Cormac Toher, Corey Oses, Mojtaba Samiee, Jon-Paul Maria, Donald W. Brenner, Kenneth S. Vecchio & Stefano Curtarolo
† contributed equally
**DOI**: 10.1038/s41467-018-07160-7

*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 Žic, 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

## 2019

*Book Chapter* — 3

Automated computation of materials properties, *Materials Informatics: Methods, Tools and Applications*

**Authors**: Cormac Toher, Corey Oses & Stefano Curtarolo
**URL**: wiley.com/en-us/Materials+Informatics%3A+Methods%2C+Tools%2C+and+Applications-p-9783527802272

## 2018

*Book Chapter* — 2

Machine learning and high-throughput approaches to magnetism, *Handbook of Materials Modeling. Volume 2 Applications: Current and Emerging Materials*

**Authors**: Stefano Sanvito, Mario Žic, James Nelson, Thomas Archer, Corey Oses & Stefano Curtarolo
**DOI**: 10.1007/978-3-319-50257-1_108-1

*Book Chapter* — 1

The AFLOW Fleet for Materials Discovery, *Handbook of Materials Modeling. Volume 1 Methods: Theory and Modeling*

**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
**DOI**: 10.1007/978-3-319-42913-7_63-1

# 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, August 14, 2015

# Certifications

*Participant* — June 11–14, 2019 — 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* — June 25–29, 2018 — Machine Learning Summer School (MLSS) at Duke University

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| *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 |