COREY OSES

Materials Science, Duke University

Personal Information · Work Experience · Education · Press and News Releases · Honors and Awards · Workshops · Journal Publications · Book Publications · Teaching Experience · Certifications

PERSONAL INFORMATION

email corey.oses@duke.edu phone (W) +1 (919) 684 1553

website coreyoses.com

WORK EXPERIENCE

Postdoctoral Fellow 2018–present Duke University

Supervisor: S. Curtarolo

Internship Summer 2013 Cornell High Energy Synchrotron Source (BioSAXS on F2 and G

Beamlines)
Supervisors: R. E. Gillilan & E. Fontes

Internship Summer 2012 Cornell High Energy Synchrotron Source (Capillary Optics Group)

Supervisors: R. Huang & E. 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: S. Curtarolo

B.Sc. 2009–2013 Cornell University

Department: Applied and Engineering Physics

Thesis: Plume Propagation Simulation for Pulsed Laser Deposition

Advisor: J. Brock

PRESS AND NEWS RELEASES

Duke University November 2018 "Disordered Materials Could Be Hardest, Most Heat-Tolerant Ever"

Pratt School of Engineering

• This press release is featured on AAAS EurekAlert!, Phys.org, ScienceDaily, Science Bulletin, Naaju,

NewsBeezer, RemoNews, Tech2, and LongRoom News.

MRS Bulletin August 2017 "Universal fragment descriptor predicts materials properties"

cambridge.org/core/journals/mrs-bulletin/news/universal-fragment-descriptor-predicts-materials-predicts-ma

properties

UNC Eshelman June 2017 "Breakthrough Tool Predicts Properties of Theoretical Materials, Finds

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

School of Pharmacy

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 April 2017 "Computers Create Recipe for Two New Magnetic Materials"

Pratt School of Engineering

 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

Computational Chemistry Highlights	compchemhighlight	"Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints" our de force for computational materials science" — Prof. Aspuru-Guzik. s.org/2015/01/materials-cartography-representing-and.html
Duke University Research	January 2015 research.duke.edu/1	"Molecular Tornado" molecular-tornado
Duke University Graduate School	October 2014 gradschool.duke.edu	"Competing for NSF Fellowships: Advice from a Current Fellow" u/professional-development/blog/competing-nsf-fellowships-advice-current-fellow
ERN Conference 2013	February 2013 new.emerging-resear	"2013 Oral and Poster Presentation Award Winners" rchers.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	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

WORKSHOPS

Organizer And Presenter

2020 AFLOW School: Integrated infrastructure for computational materials discovery

Co-Organizers: C. Toher, D. Hicks, M. Esters, E. Gossett, R. Friedrich, M. J. Brenner & S. Curtarolo

- 8. **Presenter** at the Dresden Center for Computational Materials Science (DCMS) Materials 4.0 Summer School 2020, Technische Universität Dresden August 18, 2020.
 - "Thermodynamics: AFLOW-CHULL" recording: youtu.be/ncm356YNBVc
- Presenter 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 — July 23, 2020.
 - "Materials Database and Machine Learning: AFLOW-ML" recording: youtu.be/x2qeBtOXues
- Organizer and presenter at the Texas A&M University AFLOW Multi-Day Workshop, College Station, Texas — June 16–18, 2020.
 - "Introduction to Density Functional Theory: VASP" recording: youtu.be/ChySAfo2w7g
 - "Thermodynamics: AFLOW-CHULL" recording: youtu.be/9Sa8D4inJ5w
 - "Disorder: AFLOW-POCC" recording: youtu.be/xr-mU-1ShQQ
- Presenter 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.
- Organizer and presenter at the University of Pennsylvania AFLOW Full-Day Workshop, Philadelphia, Pennsylvania — May 03, 2019.
- Organizer and presenter at the North Carolina State University AFLOW Full-Day Workshop, Raleigh, North Carolina — March 12, 2019.
- Organizer and presenter at the Carnegie Mellon University AFLOW Full-Day Workshop, Pittsburgh, Pennsylvania — January 21, 2019.
- Presenter 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.

JOURNAL PUBLICATIONS 2020

Under Review

6 Carbon Stoichiometry and Mechanical Properties of High Entropy Carbide

Authors: M. D. Hossain[†], T. Borman[†], F. A. Kumar, X. Chen, A. Khosravani, S. R. Kalidindi, E. A. Paisley, M. Esters, C. Oses, C. Toher, S. Curtarolo, J. M. LeBeau, D. W. Brenner & J.-P. Maria [†] contributed equally

Under Review

Toward Robot Science: Closed-Loop Autonomous System for Materials Exploration and Optimization (CAMEO)

Authors: A. G. Kusne † , H. Yu † , C. Wu, H. Zhang, J. Hattrick-Simpers, B. DeCost, S. Sarker, C. Oses, C. Toher, S. Curtarolo, A. Davidov, R. Agarwal, L. Bendersky, M. Li, A. Mehta & I. Takeuchi † contributed equally

Under Review

24 Fermi energy engineering of enhanced toughness in high entropy carbides

Authors: T. J. Harrington † , C. Oses † , C. Toher, W. M. Mellor, K. Kaufmann, J. Gild, A. Wright, J. Luo, S. Curtarolo & K. S. Vecchio † contributed equally

NPJ Computational Materials Discovery of novel high-entropy ceramics via machine learning

NPJ Comput. Mater. 6(42) (2020)

Authors: K. Kaufmann, D. Maryanovsky, W. M. Mellor, C. Zhu, A. S. Rosengarten, T. J. Harrington, C. Oses, C. Toher, S. Curtarolo & K. S. Vecchio

DOI: 10.1038/s41524-020-0317-6

Nature Reviews Materials High-entropy ceramics

Nat. Rev. Mater. 5, 295–309 (2020)

Authors: C. Oses, C. Toher & S. Curtarolo

DOI: 10.1038/s41578-019-0170-8

2019

Metallic glasses for biodegradable implants 21 Acta Materialia Acta Mater. 176, 297–305 (2019) Authors: D. C. Ford, D. Hicks, C. Oses, C. Toher & S. Curtarolo DOI: 10.1016/j.actamat.2019.07.008 Predicting Superhard Materials via a Machine Learning Informed Evolutionary NPI Computational 20 Structure Search Materials NPJ Comput. Mater. 5, 89 (2019) Authors: P. Avery, X. Wang, C. Oses, E. Gossett, D. M. Proserpio, C. Toher, S. Curtarolo & E. Zurek DOI: 10.1038/s41524-019-0226-8 *Unavoidable disorder and entropy in multi-component systems* NPI Computational 19 NPI Comput. Mater. 5, 69 (2019) Materials Authors: C. Toher, C. Oses, D. Hicks & S. Curtarolo **DOI**: 10.1038/s41524-019-0206-z Coordination corrected ab initio formation enthalpies NPI Computational NPJ Comput. Mater. 5, 59 (2019) Materials Authors: R. Friedrich, D. Usanmaz, C. Oses, A. R. Supka, M. Fornari, M. Buongiorno Nardelli, C. Toher & S. Curtarolo DOI: 10.1038/s41524-019-0192-1 AFLOW-QHA3P: Robust and automated method to compute thermodynamic properties Physical Review 17 of solids Materials Phys. Rev. Mater. 3, 073801 (2019) Authors: P. Nath, D. Usanmaz, D. Hicks, C. Oses, M. Fornari, M. Buongiorno Nardelli, C. Toher &

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: C. Oses, E. Gossett, D. Hicks, F. Rose, M. J. Mehl, E. Perim, I. Takeuchi, S. Sanvito, M. Scheffler, Y. Lederer, O. Levy, C. Toher & S. Curtarolo
DOI: 10.1021/acs.jcim.8b00393

Data-driven design of inorganic materials with the Automatic Flow Framework for
MRS Bulletin

15

Materials Discovery
MRS Bull. 43(9), 670–675 (2018)

Authors: C. Oses, C. Toher & S. 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: P. Sarker[†], T. J. Harrington[†], C. Toher, C. Oses, M. Samiee, J.-P. Maria, D. W. Brenner, K. S. Vecchio & S. Curtarolo [†] contributed equally

DOI: 10.1038/s41467-018-07160-7

NPJ Computational Materials Machine learning modeling of superconducting critical temperature

NPJ Comput. Mater. 4, 29 (2018)

Authors: V. Stanev, C. Oses, A. G. Kusne, E. Rodriguez, J. Paglione, S. Curtarolo & I. Takeuchi DOI: 10.1038/s41524-018-0085-8

Computational Materials Science AFLOW-ML: A RESTful API for machine-learning prediction of materials properties Comput. Mater. Sci. **152**, 134–145 (2018)

Authors: E. Gossett, C. Toher, C. Oses, O. Isayev, F. Legrain, F. Rose, E. Zurek, J. Carrete, N. Mingo, A. Tropsha & S. Curtarolo

• This paper was selected for Editor's Choice.

DOI: 10.1016/j.commatsci.2018.03.075

AFLOW-SYM: platform for the complete, automatic and self-consistent symmetry analysis of crystals Acta 11 Acta Cryst. A 74, 184-203 (2018) Crystallographica Section A Authors: D. Hicks, C. Oses, E. Gossett, G. Gomez, R. H. Taylor, C. Toher, M. J. Mehl, O. Levy & S. Curtarolo DOI: 10.1107/S2053273318003066 2017 The structure and composition statistics of 6A binary and ternary structures Inorganic 10 Inorg. Chem. 57(2), 653–667 (2017) Chemistry Authors: A. Hever, C. Oses, S. Curtarolo, O. Levy & A. Natan DOI: 10.1021/acs.inorgchem.7b02462 AFLUX: The LUX materials search API for the AFLOW data repositories Computational Comput. Mater. Sci. 137, 362–370 (2017) Materials Science Authors: F. Rose, C. Toher, E. Gossett, C. Oses, M. Buongiorno Nardelli, M. Fornari & S. Curtarolo • This paper was selected for Editor's Choice. DOI: 10.1016/j.commatsci.2017.04.036 Universal Fragment Descriptors for Predicting Properties of Inorganic Crystals Nature Nat. Commun. 8, 15679 (2017) Communications **Authors**: O. Isayev[†], C. Oses[†], C. Toher, E. Gossett, S. Curtarolo & A. Tropsha † contributed equally DOI: 10.1038/ncomms15679 Combining the AFLOW GIBBS and elastic Libraries to efficiently and robustly screening Physical Review 7 thermomechanical properties of solids Materials Phys. Rev. Mater. 1, 015401 (2017) Authors: C. Toher, C. Oses, J. J. Plata, D. Hicks, F. Rose, O. Levy, M. de Jong, M. Asta, M. Fornari, M. Buongiorno Nardelli & S. Curtarolo DOI: 10.1103/PhysRevMaterials.1.015401 A Computational High-Throughput Search for New Ternary Superalloys Acta Materialia 6 Acta Mater. 122, 438-447 (2017) Authors: C. Nyshadham, C. Oses, J. E. Hansen, I. Takeuchi, S. Curtarolo & G. L. Hart DOI: 10.1016/j.actamat.2016.09.017 Accelerated Discovery of New Magnets in the Heusler Alloy Family Science Advances 5 Sci. Adv. 3(4), e1602241 (2017) Authors: S. Sanvito, C. Oses, J. Xue, A. Tiwari, M. Žic, T. Archer, P. Tozman, M. Venkatesan, J. D. Coey & S. Curtarolo DOI: 10.1126/sciadv.1602241 2016 High-Throughput Computation of Thermal Conductivity of High-Temperature Solid Physical Review X 4 Phases: The Case of Oxide and Fluoride Perovskites Phys. Rev. X 6(4), 041061 (2016) Authors: A. van Roekeghem, J. Carrete, C. Oses, S. Curtarolo & N. Mingo

DOI: 10.1103/PhysRevX.6.041061

Chemistry of Materials

Modeling Off-Stoichiometry Materials with a High-Throughput Ab-Initio Approach 3 Chem. Mater. 28(18), 6484-6492 (2016)

Authors: K. Yang, C. Oses & S. Curtarolo DOI: 10.1021/acs.chemmater.6b01449

2015

Computational Materials Science

The AFLOW Standard for High-Throughput Materials Science Calculations 2 Comput. Mater. Sci. 108A, 233-238 (2015)

Authors: C. E. Calderon, J. J. Plata, C. Toher, C. Oses, O. Levy, M. Fornari, A. Natan, M. J. Mehl, G. L. Hart, M. Buongiorno Nardelli & S. Curtarolo

• This paper was selected for Editor's Choice.

DOI: 10.1016/j.commatsci.2015.07.019

Materials Cartography: Representing and Mining Materials Space Using Structural

Chemistry of Materials

Book Chapter

and Electronic Fingerprints 1

Chem. Mater. **27**(3), 735–743 (2015)

Authors: O. Isayev, D. Fourches, E. N. Muratov, C. Oses, K. M. Rasch, A. Tropsha & S. Curtarolo

• This paper was selected for Editor's Choice.

DOI: 10.1021/cm503507h

BOOK PUBLICATIONS

2019

Automated computation of materials properties

Materials Informatics: Methods, Tools and Applications, Ch. 7

Authors: C. Toher, C. Oses & S. Curtarolo

URL: wiley.com/en-us/Materials+Informatics%3A+Methods%2C+Tools%2C+and+Applications-p-

9783527802272

2018

Machine learning and high-throughput approaches to magnetism

Handbook of Materials Modeling. Volume 2 Applications: Current and **Book Chapter** 2

Emerging Materials

Authors: S. Sanvito, M. Žic, J. Nelson, T. Archer, C. Oses & S. Curtarolo

DOI: 10.1007/978-3-319-50257-1_108-1

Book Chapter

The AFLOW Fleet for Materials Discovery

Handbook of Materials Modeling. Volume 1 Methods: Theory and Modeling

Authors: C. Toher, C. Oses, D. Hicks, E. Gossett, F. Rose, P. Nath, D. Usanmaz, D. C. Ford, E. Perim, C. E. Calderon, J. J. Plata, Y. Lederer, M. Jahnátek, W. Setyawan, S. Wang, J. Xue, K. M. Rasch, R. V. Chepulskii, R. H. Taylor, G. Gomez, H. Shi, A. R. Supka, R. Al Rahal Al Orabi, P. Gopal, F. T. Cerasoli, L. Liyanage, H. Wang, I. Siloi, L. A. Agapito, C. Nyshadham, G. L. Hart, J. Carrete, F. Legrain, N. Mingo, E. Zurek, O. Isayev, A. Tropsha, S. Sanvito, R. M. Hanson, I. Takeuchi, M. J. Mehl, A. N. Kolmogorov, K. Yang, P. D'Amico, A. Calzolari, M. Costa, R. De Gennaro, M. Buongiorno Nardelli, M. Fornari, O. Levy & S. Curtarolo

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

TEACHING EXPERIENCE

ME 555: Computational Materials Science by Examples and

CECAM (Centre Européen de Calcul Atomique et Moléculaire)

Duke University Department of Mechanical Teaching Assistant Applications, Spring 2020

Engineering and Materials Science

ME 221: Structure and Properties of Solids, Duke University Fall 2014–Spring Teaching Assistant

Department of Mechanical Engineering and Materials Science

• Best Teaching Assistant Award, August 14, 2015

CERTIFICATIONS

Open Databases Integration for Materials Design (OPTiMaDe) Participant June 8-12, 2020 Workshop at the École polytechnique fédérale de Lausanne (EPFL) CECAM (Centre Européen de Calcul Atomique et Moléculaire) Participant June 11-14, 2019 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 CECAM (Centre Européen de Calcul Atomique et Moléculaire) Open Databases Integration for Materials Design (OPTiMaDe) **Participant** June 11–15, 2018 Workshop at the École polytechnique fédérale de Lausanne (EPFL) Machine Learning Summer School (MLSS) at the University of Texas

January 7–16, Graduate 2015

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