COREY OSES

Materials Science, Duke University

PERSONAL INFORMATION

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phone	(W) +1 (919) 684 1553
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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 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

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. Aspuru-Guzik. 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	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.
   - "AFLOW-CHULL: Thermodynamics" recording: youtu.be/9Sa8D4inJ5w

7. **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

6. **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
   - "AFLOW-CHULL: Thermodynamics" recording: youtu.be/9Sa8D4inJ5w
   - "AFLOW-POCC: Disorder" recording: youtu.be/xr-mU-1ShQQ

5. **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.

4. **Organizer and presenter** at the University of Pennsylvania AFLOW Full-Day Workshop, Philadelphia, Pennsylvania — May 03, 2019.

3. **Organizer and presenter** at the North Carolina State University AFLOW Full-Day Workshop, Raleigh, North Carolina — March 12, 2019.

2. **Organizer and presenter** at the Carnegie Mellon University AFLOW Full-Day Workshop, Pittsburgh, Pennsylvania — January 21, 2019.

1. **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.

J O U R N A L P U B L I C A T I O N S

2020

Under Review	25	*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	23	*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	22	*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

Acta Materialia	21	*Metallic glasses for biodegradable implants* 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

NPJ Computational Materials	20	*Predicting Superhard Materials via a Machine Learning Informed Evolutionary Structure Search* NPJ Comput. Mater. **5**, 89 (2019)

Authors: P. Avery, X. Wang, C. Oses, E. Gossett, D. M. Proserpio, C. Toher, S. Curtarolo & E. Zurek

NPJ Computational Materials	19	*Unavoidable disorder and entropy in multi-component systems* NPJ Comput. Mater. **5**, 69 (2019)

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

NPJ Computational Materials	18	*Coordination corrected ab initio formation enthalpies* NPJ Comput. Mater. **5**, 59 (2019)

Authors: R. Friedrich, D. Usanmaz, C. Oses, A. R. Supka, M. Fornari, M. Buongiorno Nardelli, C. Toher & S. Curtarolo

Physical Review Materials	17	*AFLOW-QHA3P: Robust and automated method to compute thermodynamic properties of solids* Phys. Rev. Mater. **3**, 073801 (2019)

Authors: P. Nath, D. Usanmaz, D. Hicks, C. Oses, M. Fornari, M. Buongiorno Nardelli, C. Toher & S. Curtarolo

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

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

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. Maria, D. W. Brenner, K. S. Vecchio & S. Curtarolo
[†] contributed equally

NPJ Computational Materials	13	*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

Computational Materials Science	12	*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.

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: D. Hicks, C. Oses, E. Gossett, G. Gomez, R. H. Taylor, C. Toher, M. J. Mehl, O. Levy & S. Curtarolo

2017

Inorganic Chemistry   10

The structure and composition statistics of 6A binary and ternary structures
Inorg. Chem. **57**(2), 653–667 (2017)

Authors: A. Hever, C. Oses, S. Curtarolo, O. Levy & A. 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: 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

Nature Communications   8

Universal Fragment Descriptors for Predicting Properties of Inorganic Crystals
Nat. Commun. **8**, 15679 (2017)

Authors: O. Isayev[†], C. Oses[†], C. Toher, E. Gossett, S. Curtarolo & A. 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: 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

Acta Materialia   6

A Computational High-Throughput Search for New Ternary Superalloys
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

Science Advances   5

Accelerated Discovery of New Magnets in the Heusler Alloy Family
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

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: A. van Roekeghem, J. Carrete, C. Oses, S. Curtarolo & N. 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: K. Yang, C. Oses & S. 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: 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

Chemistry of Materials	1	*Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints* 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.

BOOK PUBLICATIONS

2019

Book Chapter	3	*Automated computation of materials properties* Materials Informatics: Methods, Tools and Applications, Ch. 7

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

2018

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

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

Book Chapter	1	*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

TEACHING EXPERIENCE

Teaching Assistant	Spring 2020	ME 555: Computational Materials Science by Examples and Applications, Duke University Department of Mechanical Engineering and Materials Science
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 8–12, 2020	CECAM (Centre Européen de Calcul Atomique et Moléculaire) Open Databases Integration for Materials Design (OPTiMaDe) Workshop at the École polytechnique fédérale de Lausanne (EPFL)
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
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