# COREY OSES

Materials Science, Duke University

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

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Google Scholar user=Za7m4CMAAAAJ · citations: 1995 (YTD 638) · h-index: 20

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

Department: Mechanical Engineering and Materials Science

Thesis: Machine learning, phase stability, and disorder with the Automatic Flow Framework for Materials Discovery

DukeSpace: hdl.handle.net/10161/18254

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

University of

Buffalo

September 2019 "Scientists predict new forms of superhard carbon"

• This press release is featured on Phys.org, ScienceDaily, SciTechDaily, and Tribonet.

buffalo.edu/ubnow/stories/2019/09/zurek-superhard-carbon.html

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.

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-descriptor-predicts-descripto

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

April 2017

7 "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 January 2015 "Materials Cartography: Representing and Mining Materials Space Using

Chemistry

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 January 2015 "Molecular Tornado"

Research research.duke.edu/molecular-tornado

Duke University October 2014 "Competing for NSF Fellowships: Advice from a Current Fellow"

 ${\it Graduate School} \qquad {\it gradschool.} \\ {\it duke.edu/professional-development/blog/competing-nsf-fellowships-advice-current-fell$ 

ERN Conference February 2013 "2013 Oral and Poster Presentation Award Winners"

2013 new.emerging-researchers.org/2013-oral-and-poster-presentation-winners

# HONORS AND AWARDS

Editor's Choice, Publication in Comput. Mater. Sci., Elsevier
 Editor's Choice, Publication in Comput. Mater. Sci., Elsevier

August 14, 2015

Best Teaching Assistant Award (ME 221), Duke University Department of Mechanical

**Engineering and Materials Science** 

2015 Editor's Choice, Publication in Comput. Mater. Sci., Elsevier

2015 Editor's Choice, Publication in Chem. Mater., American Chemical Society

2013–2016 Graduate Research Fellowship, National Science Foundation

August 22, 2013

Best Presentation Award at the MEMS Departmental Retreat, Duke University

Department of Mechanical Engineering and Materials Science

March 02, 2013 First Place in Nanoscience and Physics Research Presentation, NSF / AAAS / EHR

**Emerging Researchers National Conference** 

2011–2013 Shell Incentive Fund Scholarship2010 & 2011 Xerox Corporation Scholarship

2010 & 2011 Intel Academic Award

June 18, 2010 Cornell University Unmanned Air Systems Team awarded \$1,000 grant, AUVSI

Student Unmanned Aerial Systems Competition

2009–2013 Meinig Family Cornell National Scholars

#### WORKSHOPS

AFLOW School: Integrated infrastructure for computational materials discovery

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

- 12. **Organizer and presenter** at the University of Virginia AFLOW Full-Day Workshop, Charlottesville, Virginia August 17, 2021.
  - "Thermodynamics: AFLOW-CHULL and AFLOW-CCE" recording: https://youtu.be/cLhOcN1sQ7M
- Presenter at the NIST/Moore Foundation/University of Maryland Machine Learning for Materials Research Bootcamp 2021 & Workshop on Machine Learning Quantum Materials, Institute for Bioscience & Biotechnology Research in Gaithersburg, Maryland — July 29, 2021.
  - "Materials Database and Machine Learning: AFLOW-ML" recording: https://youtu.be/uFQ-lyTaxCc
- Organizer and presenter at the Texas A&M University AFLOW Multi-Day Workshop, College Station, Texas July 12–15, 2021.
  - "Introduction to Density Functional Theory: VASP" recording: https://youtu.be/KXnJGdVgosA
  - "Thermodynamics: AFLOW-CHULL and AFLOW-CCE" recording: https://youtu.be/ElaniAcrbhU
  - "Disorder: AFLOW-POCC" recording: https://youtu.be/D\_cfHllpBiA
- 9. Session Chair of the Materials Research Society Virtual Spring Meeting Tutorial April 17, 2021.
- 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: https://youtu.be/ncm356YNBVc
- 7. **Presenter** at the NIST/Moore Foundation/University of Maryland Machine Learning for Materials Research Bootcamp 2020 & 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: https://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: https://youtu.be/ChySAfo2w7g
  - "Thermodynamics: AFLOW-CHULL" recording: https://youtu.be/9Sa8D4inJ5w
  - "Disorder: AFLOW-POCC" recording: https://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.
- $4. \ \ \, \textbf{Organizer and presenter} \ \text{at the University of Pennsylvania} \ AFLOW \ \text{Full-Day Workshop, Philadelphia, Pennsylvania} \ -- \ \text{May} \\ \ 03,2019.$
- 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.
- 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

### 2021

- 31. M. Esters, C. Oses, D. Hicks, M. J. Mehl, M. Jahnátek, M. D. Hossain, J.-P. Maria, D. W. Brenner, C. Toher & S. Curtarolo, Settling the matter of the role of vibrations in the stability of high-entropy carbides, under review.
- 30. M. D. Hossain, T. Borman, C. Oses, M. Esters, C. Toher, L. Feng, A. Kumar, W. G. Fahrenholtz, S. Curtarolo, D. W. Brenner, J. M. LeBeau & J.-P. Maria, *Entropy Landscaping of High-Entropy Carbides*, Adv. Mater. in press (2021).
- 29. D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. Hart, C. Toher & S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. in press (2021). DOI: 10.1016/j.commatsci.2021.110450.
- 28. C. W. Andersen, R. Armiento, E. Blokhin, G. J. Conduit, S. Dwaraknath, M. L. Evans, Á. Fekete, A. Gopakumar, S. Gražulis, A. Merkys, F. Mohamed, C. Oses, G. Pizzi, G.-M. Rignanese, M. Scheidgen, L. Talirz, C. Toher, D. Winston, R. Aversa, K. Choudhary, P. Colinet, S. Curtarolo, D. Di Stefano, C. Draxl, S. Er, M. Esters, M. Fornari, M. Giantomassi, M. Govoni, G. Hautier, V. Hegde, M. K. Horton, P. Huck, G. Huhs, J. Hummelshøj, A. Kariryaa, B. Kozinsky, S. Kumbhar, M. Liu, N. Marzari, A. J. Morris, A. Mostofi, K. A. Persson, G. Petretto, T. Purcell, F. Ricci, F. Rose, M. Scheffler, D. Speckhard, M. Uhrin, A. Vaitkus, P. Villars, D. Waroquiers, C. Wolverton, M. Wu & X. Yang, OPTIMADE: an API for exchanging materials data, Sci. Data 8, 217 (2021). DOI: 10.1038/s41597-021-00974-z.
- 27. R. Friedrich, M. Esters, C. Oses, S. Ki, M. J. Brenner, D. Hicks, M. J. Mehl, C. Toher & S. Curtarolo, *Automated coordination corrected enthalpies with AFLOW-CCE*, Phys. Rev. Mater. 5, 043803 (2021). DOI: 10.1103/PhysRevMaterials.5.043803.
- M. J. Mehl, M. Ronquillo, D. Hicks, M. Esters, C. Oses, R. Friedrich, A. Smolyanyuk, E. Gossett, D. Finkenstadt & S. Curtarolo, Tin-pest problem as a test of density functionals using high-throughput calculations, Phys. Rev. Mater. 5, 083608 (2021).
   DOI: 10.1103/PhysRevMaterials.5.083608.
- 25. M. D. Hossain, T. Borman, 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, *Carbon Stoichiometry and Mechanical Properties of High Entropy Carbides*, Acta Mater. 215, 117051 (2021). DOI: 10.1016/j.actamat.2021.117051.

#### 2020

- 24. A. G. Kusne, H. Yu, C. Wu, H. Zhang, J. Hattrick-Simpers, B. DeCost, S. Sarker, C. Oses, C. Toher, S. Curtarolo, A. V. Davydov, R. Agarwal, L. A. Bendersky, M. Li, A. Mehta & I. Takeuchi, *On-the-fly Closed-loop Autonomous Materials Discovery via Bayesian Active Learning*, Nat. Commun. 11, 5966 (2020). DOI: 10.1038/s41467-020-19597-w.
- K. Kaufmann, D. Maryanovsky, W. M. Mellor, C. Zhu, A. S. Rosengarten, T. J. Harrington, C. Oses, C. Toher, S. Curtarolo & K. S. Vecchio, *Discovery of novel high-entropy ceramics via machine learning*, NPJ Comput. Mater. 6, 42 (2020). DOI: 10.1038/s41524-020-0317-6.
- 22. C. Oses, C. Toher & S. Curtarolo, High-entropy ceramics, Nat. Rev. Mater. 5, 295–309 (2020). DOI: 10.1038/s41578-019-0170-8.

### 2019

- 21. D. C. Ford, D. Hicks, C. Oses, C. Toher & S. Curtarolo, Metallic glasses for biodegradable implants, Acta Mater. 176, 297–305 (2019). DOI: 10.1016/j.actamat.2019.07.008.
- 20. P. Avery, X. Wang, C. Oses, E. Gossett, D. M. Proserpio, C. Toher, S. Curtarolo & E. Zurek, *Predicting Superhard Materials via a Machine Learning Informed Evolutionary Structure Search*, NPJ Comput. Mater. **5**, 89 (2019). **DOI**: 10.1038/s41524-019-0226-8.
- 19. C. Toher, C. Oses, D. Hicks & S. Curtarolo, *Unavoidable disorder and entropy in multi-component systems*, NPJ Comput. Mater. 5, 69 (2019). **DOI**: 10.1038/s41524-019-0206-z.
- 18. R. Friedrich, D. Usanmaz, C. Oses, A. R. Supka, M. Fornari, M. Buongiorno Nardelli, C. Toher & S. Curtarolo, *Coordination corrected ab initio formation enthalpies*, NPJ Comput. Mater. 5, 59 (2019). **DOI**: 10.1038/s41524-019-0192-1.
- 17. P. Nath, D. Usanmaz, D. Hicks, C. Oses, M. Fornari, M. Buongiorno Nardelli, C. Toher & S. Curtarolo, *AFLOW-QHA3P: Robust and automated method to compute thermodynamic properties of solids*, Phys. Rev. Mater. **3**, 073801 (2019). **DOI:** 10.1103/PhysRevMaterials.3.073801.

#### 2018

- 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, AFLOW-CHULL: Cloud-oriented platform for autonomous phase stability analysis, J. Chem. Inf. Model. 58(12), 2477–2490 (2018). DOI: 10.1021/acs.jcim.8b00393.
- 15. C. Oses, C. Toher & S. Curtarolo, *Data-driven design of inorganic materials with the Automatic Flow Framework for Materials Discovery*, MRS Bull. **43**(9), 670–675 (2018). **DOI**: 10.1557/mrs.2018.207.
- P. Sarker, T. J. Harrington, C. Toher, C. Oses, M. Samiee, J.-P. Maria, D. W. Brenner, K. S. Vecchio & S. Curtarolo, Novel high-entropy high-hardness metal carbides discovered by entropy descriptors, Nat. Commun. 9, 4980 (2018). DOI: 10.1038/s41467-018-07160-7.
- 13. V. Stanev, C. Oses, A. G. Kusne, E. Rodriguez, J. Paglione, S. Curtarolo & I. Takeuchi, *Machine learning modeling of superconducting critical temperature*, NPJ Comput. Mater. **4**, 29 (2018). **DOI**: 10.1038/s41524-018-0085-8.
- 12. E. Gossett, C. Toher, C. Oses, O. Isayev, F. Legrain, F. Rose, E. Zurek, J. Carrete, N. Mingo, A. Tropsha & S. Curtarolo, *AFLOW-ML: A RESTful API for machine-learning prediction of materials properties*, Comput. Mater. Sci. **152**, 134–145 (2018). **DOI:** 10.1016/j.commatsci.2018.03.075.
  - This paper was selected for Editor's Choice.
- 11. D. Hicks, C. Oses, E. Gossett, G. Gomez, R. H. Taylor, C. Toher, M. J. Mehl, O. Levy & S. Curtarolo, *AFLOW-SYM: platform for the complete, automatic and self-consistent symmetry analysis of crystals,* Acta Cryst. A **74**, 184–203 (2018). **DOI:** 10.1107/S2053273318003066.

#### 2017

- 10. A. Hever, C. Oses, S. Curtarolo, O. Levy & A. Natan, *The structure and composition statistics of 6A binary and ternary structures*, Inorg. Chem. 57(2), 653–667 (2017). **DOI:** 10.1021/acs.inorgchem.7b02462.
- 9. F. Rose, C. Toher, E. Gossett, C. Oses, M. Buongiorno Nardelli, M. Fornari & S. Curtarolo, *AFLUX: The LUX materials search API for the AFLOW data repositories*, Comput. Mater. Sci. 137, 362–370 (2017). DOI: 10.1016/j.commatsci.2017.04.036.
  - This paper was selected for Editor's Choice.
- 8. O. Isayev, C. Oses, C. Toher, E. Gossett, S. Curtarolo & A. Tropsha, *Universal Fragment Descriptors for Predicting Properties of Inorganic Crystals*, Nat. Commun. **8**, 15679 (2017). **DOI**: 10.1038/ncomms15679.
- 7. 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, *Combining the AFLOW GIBBS and elastic libraries to efficiently and robustly screening thermomechanical properties of solids*, Phys. Rev. Mater. 1, 015401 (2017). DOI: 10.1103/PhysRevMaterials.1.015401.
- 6. C. Nyshadham, C. Oses, J. E. Hansen, I. Takeuchi, S. Curtarolo & G. L. Hart, *A Computational High-Throughput Search for New Ternary Superalloys*, Acta Mater. **122**, 438–447 (2017). **DOI**: 10.1016/j.actamat.2016.09.017.
- 5. S. Sanvito, C. Oses, J. Xue, A. Tiwari, M. Žic, T. Archer, P. Tozman, M. Venkatesan, J. D. Coey & S. Curtarolo, *Accelerated Discovery of New Magnets in the Heusler Alloy Family*, Sci. Adv. 3(4), e1602241 (2017). DOI: 10.1126/sciadv.1602241.

#### 2016

- 4. A. van Roekeghem, J. Carrete, C. Oses, S. Curtarolo & N. Mingo, *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). **DOI**: 10.1103/PhysRevX.6.041061.
- 3. K. Yang, C. Oses & S. Curtarolo, *Modeling Off-Stoichiometry Materials with a High-Throughput Ab-Initio Approach*, Chem. Mater. **28**(18), 6484–6492 (2016). **DOI**: 10.1021/acs.chemmater.6b01449.

#### 2015

- 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, *The AFLOW Standard for High-Throughput Materials Science Calculations*, Comput. Mater. Sci. 108A, 233–238 (2015). DOI: 10.1016/j.commatsci.2015.07.019.
  - This paper was selected for Editor's Choice.
- O. Isayev, D. Fourches, E. N. Muratov, C. Oses, K. M. Rasch, A. Tropsha & S. Curtarolo, Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints, Chem. Mater. 27(3), 735–743 (2015). DOI: 10.1021/cm503507h.
  - This paper was selected for Editor's Choice.

# BOOK PUBLICATIONS

## 2019

3. C. Toher, C. Oses & S. Curtarolo, *Automated computation of materials properties*, Materials Informatics: Methods, Tools and Applications, Ch. 7. URL: wiley.com/en-us/Materials+Informatics%3A+Methods%2C+Tools%2C+and+Applications-p-9783527802272.

#### 2018

- S. Sanvito, M. Žic, J. Nelson, T. Archer, C. Oses & S. Curtarolo, Machine learning and high-throughput approaches to magnetism, Handbook of Materials Modeling. Volume 2 Applications: Current and Emerging Materials. DOI: 10.1007/978-3-319-50257-1 108-1.
- 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, *The AFLOW Fleet for Materials Discovery*, Handbook of Materials Modeling. Volume 1 Methods: Theory and Modeling. DOI: 10.1007/978-3-319-42913-7\_63-1.

#### TEACHING EXPERIENCE

Co-Instructor	Spring 2021	ME 555: Applications of Artificial Intelligence in Materials, Duke University Department of Mechanical Engineering and Materials Science
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 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
Technician License	July 29, 2010	American Radio Relay League (ARRL) in Roselle, New Jersey