COREY OSES

Materials Science, Duke University

PERSONAL INFORMATION

corey.oses@duke.edu email

 $(M) +1 (201) 674 1407 \cdot (W) +1 (919) 684 1553$ phone

website coreyoses.com

WORK EXPERIENCE

Postdoctoral Fellow 2018-present **Duke University**

Supervisor: S. Curtarolo

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

Beamlines)

Supervisors: R. E. Gillilan & E. Fontes

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

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

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

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

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

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

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

"Materials fingerprints identified for informatics" MRS Bulletin April 2015

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"

Graduate School gradschool.duke.edu/professional-development/blog/competing-nsf-fellowships-advice-current-fellow

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, 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
- 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
 - "Thermodynamics: AFLOW-CHULL" recording: youtu.be/9Sa8D4inJ5w
 - "Disorder: AFLOW-POCC" 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.
- 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.
- 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.

TALKS / PRESENTATIONS

High-entropy ceramics

23. **Invited seminar** at the North Carolina State University Lecture Series in Materials Science & Engineering, Raleigh, North Carolina — January 22, 2021.

Entropy and ceramics: A valuable partnership

- 22. **Invited seminar** at the Weizmann Institute of Science Department of Materials and Interfaces Seminar, Rehovot, Israel February 06, 2020.
- 21. **Invited seminar** at the Tel Aviv University Sackler Center for Computational Molecular and Materials Science Seminar, Tel Aviv, Israel February 05, 2020.
- 20. **Invited seminar** at the Ben-Gurion University of the Negev Materials Science Department Seminar, Beer Sheva, Israel January 29, 2020.

Cloud-oriented computational phase diagrams with AFLOW-CHULL

- 19. Contributed talk at the American Physical Society March Meeting, Boston, Massachusetts March 07, 2019.
- 18. **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.

Going Off-Stoichiometry: Challenging Traditional Materials Discovery

17. **Invited talk** at the Naval Research Laboratory Center for Computational Materials Science Seminar, Washington, D.C. — January 09, 2019.

Universal Fragment Descriptors for Predicting Properties of Inorganic Crystals

- 16. **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.
- 15. Contributed talk at the Hopkins Extreme Materials Institute Mach Conference, Annapolis, Maryland April 05, 2018.
- 14. **Contributed talk** at the Duke University Chemistry Department Third Annual Graduate Research Symposium, Durham, North Carolina October 09, 2017.
- 13. Contributed talk at the American Physical Society March Meeting, New Orleans, Louisiana March 14, 2017.

Advancements in Materials Informatics with AFLOW

- 12. **Invited talk** at the Fritz-Haber-Institut der Max-Planck-Gesellschaft Theory Department Seminar, Berlin, Germany January 18, 2018.
- 11. Invited talk at the Humboldt University of Berlin Physics Department Seminar, Berlin, Germany January 16, 2018.

Modeling Off-Stoichiometric Materials with a High-Throughput, Ab-Initio Approach

10. Contributed talk at the American Physical Society March Meeting, Baltimore, Maryland — March 16, 2016.

Materials Cartography: Representing and Mining Materials Space using Structural and Electronic Fingerprints

- 9. Invited talk at the Brigham Young University Condensed Matter Physics Seminar, Provo, Utah February 18, 2016.
- 8. **Contributed talk** at the Duke Mechanical Engineering and Materials Science (MEMS) Department Graduate Student Seminar, Durham, North Carolina September 25, 2015.
- 7. Contributed talk at the American Physical Society March Meeting, San Antonio, Texas March 02, 2015.

Plume Propagation Simulation for Pulsed Laser Deposition

- 6. **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.
- 4. **Poster presentation** at the MRS / ASM / AVS / AReMS Meeting, North Carolina State University, Raleigh, North Carolina November 15, 2013.
- 3. **Poster presentation** at the Duke Mechanical Engineering and Materials Science (MEMS) Department Annual Retreat, Durham, North Carolina August 22, 2013.
 - Best Presentation Award

Synchrotron Radiation Focusing Optics — Capillary Beam Stop Design

- 2. 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
- 1. Poster presentation at the Cornell University Chapter of LSAMP Research Symposium, Ithaca, New York August 07, 2012.

JOURNAL PUBLICATIONS

2021

- 29. 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*, under review. arXiv: arxiv:2101.02724.
- 28. 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*, under review. arXiv: arxiv:2012.05961.
- 27. M. J. Mehl, M. Ronquillo, D. Hicks, M. Esters, C. Oses, R. Friedrich, A. Smolyanyuk, E. Gossett, D. Finkenstadt & S. Curtarolo, *The Tin Pest Problem as a Test of Density Functionals Using High-Throughput Calculations*, under review. arXiv: arxiv:2010.07168.
- 26. 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, *Carbon Stoichiometry and Mechanical Properties of High Entropy Carbide*, under review.
 - † contributed equally 5. T. J. Harrington[†], C. Oses[†], C. Toher, W. M
- 25. T. J. Harrington[†], C. Oses[†], C. Toher, W. M. Mellor, K. Kaufmann, J. Gild, A. Wright, J. Luo, S. Curtarolo & K. S. Vecchio, *Fermi* energy engineering of enhanced toughness in high entropy carbides, under review.

 † contributed equally

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.

 † contributed equally
- 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.
 † contributed equally
- 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.
- 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.
 † contributed equally
- 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.
- 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

- 2. 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

		ME 555: Computational Materials Science by Examples and
Teaching Assistant	Spring 2020	Applications, Duke University Department of Mechanical
		Engineering and Materials Science
Teaching Assistant	Fall 2014–Spring	ME 221: Structure and Properties of Solids, Duke University
	2015	Department of Mechanical Engineering and Materials Science
	Best Teaching Ass	istant 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