COREY OSES

Materials Science, Duke University

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*
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

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

2018	Editor's Choice, Publication in Comput. Mater. Sci., Elsevier
2017	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 Scholarship
2010 & 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.
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.

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
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
23. 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

16. 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.
14. 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.
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.
    † 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.
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

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.
1. 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

2. 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.
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

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
Technician License	July 29, 2010	American Radio Relay League (ARRL) in Roselle, New Jersey