

# COREY OSES

Materials Science, Duke University

## PERSONAL INFORMATION

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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  
**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](https://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](http://Phys.org), [ScienceDaily](http://ScienceDaily), [SciTechDaily](http://SciTechDaily), and [Tribonet](http://Tribonet).  
[buffalo.edu/ubnow/stories/2019/09/zurek-superhard-carbon.html](http://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 EurekaAlert!](http://AAAS EurekaAlert!), [Phys.org](http://Phys.org), [ScienceDaily](http://ScienceDaily), [Science Bulletin](http://Science Bulletin), [Naaju](http://Naaju), [NewsBeezer](http://NewsBeezer), [RemoNews](http://RemoNews), [Tech2](http://Tech2), and [LongRoom News](http://LongRoom News).  
[pratt.duke.edu/about/news/chaotic-carbides](http://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](http://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 EurekaAlert!](http://AAAS EurekaAlert!), [Phys.org](http://Phys.org), and [ScienceDaily](http://ScienceDaily).  
[pharmacy.unc.edu/news/2017/06/06/breakthrough-tool-predicts-properties-theoretical-materials-finds-new-uses-current-ones/](http://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](http://Phys.org), [Slashdot](http://Slashdot), [Hacker News](http://Hacker News), [Reddit](http://Reddit), [Engadget](http://Engadget), [Engineering.com](http://Engineering.com), [Science Alert](http://Science Alert), [Azo Materials](http://Azo Materials), [Next Big Future](http://Next Big Future), [Futurism](http://Futurism), [New Atlas](http://New Atlas), and [International Business Times](http://International Business Times).  
[pratt.duke.edu/about/news/predicting-magnets](http://pratt.duke.edu/about/news/predicting-magnets)

*MRS Bulletin* April 2015 “*Materials fingerprints identified for informatics*”  
[doi.org/10.1557/mrs.2015.76](https://doi.org/10.1557/mrs.2015.76)

Computational Chemistry Highlights	January 2015	<i>"Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints"</i> • "This paper is a <i>tour de force</i> for computational materials science" — Prof. Aspuru-Guzik. <a href="http://compchemhighlights.org/2015/01/materials-cartography-representing-and.html">compchemhighlights.org/2015/01/materials-cartography-representing-and.html</a>
Duke University Research	January 2015	<i>"Molecular Tornado"</i> <a href="http://research.duke.edu/molecular-tornado">research.duke.edu/molecular-tornado</a>
Duke University Graduate School	October 2014	<i>"Competing for NSF Fellowships: Advice from a Current Fellow"</i> <a href="http://gradschool.duke.edu/professional-development/blog/competing-nsf-fellowships-advice-current-fellow">gradschool.duke.edu/professional-development/blog/competing-nsf-fellowships-advice-current-fellow</a>
ERN Conference 2013	February 2013	<i>"2013 Oral and Poster Presentation Award Winners"</i> <a href="http://new.emerging-researchers.org/2013-oral-and-poster-presentation-winners">new.emerging-researchers.org/2013-oral-and-poster-presentation-winners</a>

## HONORS AND AWARDS

2018	Editor's Choice, <i>Publication in Comput. Mater. Sci.</i> , Elsevier
2017	Editor's Choice, <i>Publication in Comput. Mater. Sci.</i> , Elsevier
August 14, 2015	<i>Best Teaching Assistant Award (ME 221)</i> , Duke University Department of Mechanical Engineering and Materials Science
2015	Editor's Choice, <i>Publication in Comput. Mater. Sci.</i> , Elsevier
2015	Editor's Choice, <i>Publication in Chem. Mater.</i> , American Chemical Society
2013–2016	Graduate Research Fellowship, National Science Foundation
August 22, 2013	<i>Best Presentation Award at the MEMS Departmental Retreat</i> , Duke University Department of Mechanical Engineering and Materials Science
March 02, 2013	<i>First Place in Nanoscience and Physics Research Presentation</i> , 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, A. Smolyanyuk, R. Friedrich, M. J. Brenner & S. Curtarolo

11. **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: [youtu.be/uFQ-lyTaxCc](https://youtu.be/uFQ-lyTaxCc)
10. **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: [youtu.be/KXnJGdVgosA](https://youtu.be/KXnJGdVgosA)
  - “Thermodynamics: AFLOW-CHULL” recording: [youtu.be/ElaniAcrbhU](https://youtu.be/ElaniAcrbhU)
  - “Disorder: AFLOW-POCC” recording: [youtu.be/D\\_cfHilpBiA](https://youtu.be/D_cfHilpBiA)
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: [youtu.be/ncm356YNBVc](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: [youtu.be/x2qeBtOXues](https://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](https://youtu.be/ChySAfo2w7g)
  - “Thermodynamics: AFLOW-CHULL” recording: [youtu.be/9Sa8D4inJ5w](https://youtu.be/9Sa8D4inJ5w)
  - “Disorder: AFLOW-POCC” recording: [youtu.be/xr-mU-1ShQQ](https://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.

## TALKS / PRESENTATIONS

### *High-entropy ceramics*

24. **Invited seminar** at the Texas A&M University Department of Mechanical Engineering Seminar, College Station, Texas — February 24, 2021.
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 seminar** 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) 13<sup>th</sup> 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 seminar** at the Fritz-Haber-Institut der Max-Planck-Gesellschaft Theory Department Seminar, Berlin, Germany — January 18, 2018.
11. **Invited seminar** 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 seminar** 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.
5. **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

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. 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 **in press** (2021). DOI: [10.1038/s41597-021-00974-z](https://doi.org/10.1038/s41597-021-00974-z).
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*, Comput. Mater. Sci. **in press** (2021). arXiv: [arxiv:2012.05961](https://arxiv.org/abs/2012.05961).
27. M. J. Mehl, M. Ronquillo, D. Hicks, M. Esters, C. Oses, R. Friedrich, A. Smolyanyuk, E. Gossett, D. Finkenshtadt & S. Curtarolo, *The Tin Pest Problem as a Test of Density Functionals Using High-Throughput Calculations*, Phys. Rev. Mater. **in press** (2021). arXiv: [arxiv:2010.07168](https://arxiv.org/abs/2010.07168).
26. 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](https://doi.org/10.1103/PhysRevMaterials.5.043803).
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](https://doi.org/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](https://doi.org/10.1038/s41467-020-19597-w).
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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://www.wiley.com/en-us/Materials+Informatics%3A+Methods%2C+Tools%2C+and+Applications-p-9783527802272).

2018

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## 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



<i>Teaching Assistant</i>	Fall 2014–Spring 2015	ME 221: Structure and Properties of Solids, Duke University Department of Mechanical Engineering and Materials Science
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- [Best Teaching Assistant Award](#), August 14, 2015

## CERTIFICATIONS

<i>Participant</i>	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)
<i>Participant</i>	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)
<i>Graduate</i>	June 25–29, 2018	Machine Learning Summer School (MLSS) at Duke University
<i>Participant</i>	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)
<i>Graduate</i>	January 7–16, 2015	Machine Learning Summer School (MLSS) at the University of Texas at Austin
<i>Graduate</i>	May 22–27, 2011	<i>The LeaderShape Institute</i> at Cornell University
<i>Technician License</i>	July 29, 2010	American Radio Relay League (ARRL) in Roselle, New Jersey