

# COREY OSES

Materials Science, Duke University

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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

## JOURNAL PUBLICATIONS

2021

34. C. Oses, D. Hicks, R. Friedrich, M. Esters, Y. Lederer, J.-P. Maria, D. W. Brenner, F. Rose, C. Toher & S. Curtarolo, *Entropy stabilization coefficient: Resolving synthesizability of high entropy ceramics*, in preparation.
33. A. G. Kusne, A. McDannald, B. DeCost, C. Oses, C. Toher, S. Curtarolo, A. Mehta & I. Takeuchi, *Physics in the Machine: Integrating Physical Knowledge in Autonomous Phase-Mapping*, under review. **arXiv:** [arxiv:2111.07478](https://arxiv.org/abs/2111.07478).
32. C. Toher, C. Oses, M. Esters, D. Hicks, G. N. Kotsonis, C. M. Rost, D. W. Brenner, J.-P. Maria & S. Curtarolo, *High-entropy ceramics: propelling applications through disorder*, under review. **arXiv:** [arxiv:2111.11519](https://arxiv.org/abs/2111.11519).
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*, Nat. Commun. **12**, 5747 (2021). **DOI:** [10.1038/s41467-021-25979-5](https://doi.org/10.1038/s41467-021-25979-5).
- This paper was selected for **Editor's Highlight** by Springer Nature (2021).
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. **33**(42), 2102904 (2021). **DOI:** [10.1002/adma.202102904](https://doi.org/10.1002/adma.202102904).
29. C. W. Andersen<sup>†</sup>, R. Armiento<sup>†</sup>, E. Blokhin<sup>†</sup>, G. J. Conduit<sup>†</sup>, S. Dwaraknath<sup>†</sup>, M. L. Evans<sup>†</sup>, Á. Fekete<sup>†</sup>, A. Gopakumar<sup>†</sup>, S. Gražulis<sup>†</sup>, A. Merkys<sup>†</sup>, F. Mohamed<sup>†</sup>, C. Oses<sup>†</sup>, G. Pizzi<sup>†</sup>, G.-M. Rignanese<sup>†</sup>, M. Scheidgen<sup>†</sup>, L. Talirz<sup>†</sup>, C. Toher<sup>†</sup>, D. Winston<sup>†</sup>, 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. Karirya, 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](https://doi.org/10.1038/s41597-021-00974-z).
- <sup>†</sup> contributed equally
28. 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).
27. 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. **199**, 110450 (2021). **DOI:** [10.1016/j.commatsci.2021.110450](https://doi.org/10.1016/j.commatsci.2021.110450).

26. M. J. Mehl, M. Ronquillo, D. Hicks, M. Esters, C. Oses, R. Friedrich, A. Smolyanyuk, E. Gossett, D. Finkenzstadt & 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](https://doi.org/10.1103/PhysRevMaterials.5.083608).
25. M. D. Hossain<sup>†</sup>, T. Borman<sup>†</sup>, 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).

<sup>†</sup> contributed equally

## 2020

24. A. G. Kusne<sup>†</sup>, H. Yu<sup>†</sup>, 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).
- <sup>†</sup> 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](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).
  - This paper was highlighted as a “hot paper” by Web of Science (Clarivate Analytics) (November 16, 2021).

## 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<sup>†</sup>, T. J. Harrington<sup>†</sup>, 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).
- <sup>†</sup> 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](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 by Elsevier (2018).
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 by Elsevier (2017).
8. O. Isayev<sup>†</sup>, C. Oses<sup>†</sup>, 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).
- <sup>†</sup> 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](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** by Elsevier (2015).
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** by the American Chemical Society (2015).

## 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

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](https://doi.org/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. Chepulska, 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](https://doi.org/10.1007/978-3-319-42913-7_63-1).

## TALKS / PRESENTATIONS

### *Data for Materials Development Platforms*

25. **Invited seminar** at the Duke University aiM Program Boot Camp and Orientation, Durham, North Carolina — August 19, 2021.
  - “Data for Materials Development Platforms” recording: <https://youtu.be/wLegemRIMpk>

### *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.

## TEACHING EXPERIENCE

<i>Co-Instructor</i>	Spring 2021	ME 555: Applications of Artificial Intelligence in Materials, Duke University Department of Mechanical Engineering and Materials Science
<i>Teaching Assistant</i>	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
		• <a href="#">Best Teaching Assistant Award</a> , August 14, 2015

## WORKSHOPS

*AFLOW School: Integrated infrastructure for computational materials discovery*

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

13. **Organizer and presenter** at the Technische Universität (TU) Dresden and Helmholtz-Zentrum Dresden-Rossendorf AFLOW Multi-Day Workshop, Technische Universität (TU) Dresden — September 6–10, 2021.
  - “Introduction to Density Functional Theory: VASP” recording: [https://youtu.be/\\_RsQH3TY7kl](https://youtu.be/_RsQH3TY7kl)
  - “Thermodynamics: AFLOW-CHULL” recording: <https://youtu.be/zcY7gTZIB-Y>
  - “Disorder: AFLOW-POCC” recording: <https://youtu.be/lcDSYiF4AS4>
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>
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: <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: <https://youtu.be/KXnJGdVgosA>
  - “Thermodynamics: AFLOW-CHULL and AFLOW-CCE” recording: <https://youtu.be/ElaniAcrbHU>
  - “Disorder: AFLOW-POCC” recording: [https://youtu.be/D\\_cfHllpBiA](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 (TU) 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>
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: <https://youtu.be/ChySAfo2w7g>
  - “Thermodynamics: AFLOW-CHULL” recording: <https://youtu.be/9Sa8D4inJ5w>
  - “Disorder: AFLOW-POCC” recording: <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.

## PRESS AND NEWS RELEASES

- |   |                   |   |
|---|-------------------|---|
| White House Office<br>of Science &<br>Technology Policy | November 18, 2021 | <i>“Featured Vignette in the November 2021 Materials Genome Initiative Strategic Plan (page 9)”</i><br><a href="https://www.mgi.gov/sites/default/files/documents/MGI-2021-Strategic-Plan.pdf">mgi.gov/sites/default/files/documents/MGI-2021-Strategic-Plan.pdf</a>  |
| University of<br>Buffalo                                | September 2019    | <i>“Scientists predict new forms of superhard carbon”</i><br>• This press release is featured on <a href="https://www.phys.org">Phys.org</a> , <a href="https://www.sciencedaily.com">ScienceDaily</a> , <a href="https://www.scitechdaily.com">SciTechDaily</a> , and <a href="https://www.tribonet.net">Tribonet</a> .<br><a href="https://buffalo.edu/ubnow/stories/2019/09/zurek-superhard-carbon.html">buffalo.edu/ubnow/stories/2019/09/zurek-superhard-carbon.html</a> |



Duke University Pratt School of Engineering	November 2018	<p><i>“Disordered Materials Could Be Hardest, Most Heat-Tolerant Ever”</i></p> <ul style="list-style-type: none"> <li>This press release is featured on <a href="#">AAAS EurekAlert!</a>, <a href="#">Phys.org</a>, <a href="#">ScienceDaily</a>, <a href="#">Science Bulletin</a>, <a href="#">Naaju, NewsBeezer</a>, <a href="#">RemoNews</a>, <a href="#">Tech2</a>, and <a href="#">LongRoom News</a>.</li> </ul> <p><a href="http://pratt.duke.edu/about/news/chaotic-carbides">pratt.duke.edu/about/news/chaotic-carbides</a></p>
MRS Bulletin	August 2017	<p><i>“Universal fragment descriptor predicts materials properties”</i></p> <p><a href="http://cambridge.org/core/journals/mrs-bulletin/news/universal-fragment-descriptor-predicts-materials-properties">cambridge.org/core/journals/mrs-bulletin/news/universal-fragment-descriptor-predicts-materials-properties</a></p>
UNC Eshelman School of Pharmacy	June 2017	<p><i>“Breakthrough Tool Predicts Properties of Theoretical Materials, Finds New Uses for Current Ones”</i></p> <ul style="list-style-type: none"> <li>This press release is featured on <a href="#">AAAS EurekAlert!</a>, <a href="#">Phys.org</a>, and <a href="#">ScienceDaily</a>.</li> </ul> <p><a href="http://pharmacy.unc.edu/news/2017/06/06/breakthrough-tool-predicts-properties-theoretical-materials-finds-new-uses-current-ones/">pharmacy.unc.edu/news/2017/06/06/breakthrough-tool-predicts-properties-theoretical-materials-finds-new-uses-current-ones/</a></p>
Duke University Pratt School of Engineering	April 2017	<p><i>“Computers Create Recipe for Two New Magnetic Materials”</i></p> <ul style="list-style-type: none"> <li>This press release is featured on <a href="#">Phys.org</a>, <a href="#">Slashdot</a>, <a href="#">Hacker News</a>, <a href="#">Reddit</a>, <a href="#">Engadget</a>, <a href="#">Engineering.com</a>, <a href="#">Science Alert</a>, <a href="#">Azo Materials</a>, <a href="#">Next Big Future</a>, <a href="#">Futurism</a>, <a href="#">New Atlas</a>, and <a href="#">International Business Times</a>.</li> </ul> <p><a href="http://pratt.duke.edu/about/news/predicting-magnets">pratt.duke.edu/about/news/predicting-magnets</a></p>
MRS Bulletin	April 2015	<p><i>“Materials fingerprints identified for informatics”</i></p> <p><a href="https://doi.org/10.1557/mrs.2015.76">doi.org/10.1557/mrs.2015.76</a></p>
Computational Chemistry Highlights	January 2015	<p><i>“Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints”</i></p> <ul style="list-style-type: none"> <li>“This paper is a <i>tour de force</i> for computational materials science” — Prof. Aspuru-Guzik.</li> </ul> <p><a href="http://compchemhighlights.org/2015/01/materials-cartography-representing-and.html">compchemhighlights.org/2015/01/materials-cartography-representing-and.html</a></p>
Duke University Research	January 2015	<p><i>“Molecular Tornado”</i></p> <p><a href="http://research.duke.edu/molecular-tornado">research.duke.edu/molecular-tornado</a></p>
Duke University Graduate School	October 2014	<p><i>“Competing for NSF Fellowships: Advice from a Current Fellow”</i></p> <p><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></p>
ERN Conference 2013	February 2013	<p><i>“2013 Oral and Poster Presentation Award Winners”</i></p> <p><a href="http://new.emerging-researchers.org/2013-oral-and-poster-presentation-winners">new.emerging-researchers.org/2013-oral-and-poster-presentation-winners</a></p>

## HONORS AND AWARDS

Publication Award	November 16, 2021	<p><i>“Hot paper”, Publication in Nat. Rev. Mater., Web of Science (Clarivate Analytics)</i></p> <ul style="list-style-type: none"> <li>Published in the past two years and received enough citations in July/August 2021 to place it in the top 0.1% of papers in the academic field of Materials Science</li> </ul>
Publication Award	2021	Editor’s Highlight, Publication in Nat. Commun., Springer Nature
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

<i>Award</i>	August 22, 2013	Best Presentation Award at the MEMS Departmental Retreat, Duke University Department of Mechanical Engineering and Materials Science
<i>Award</i>	March 02, 2013	First Place in Nanoscience and Physics Research Presentation, NSF / AAAS / EHR Emerging Researchers National Conference
<i>Scholarship</i>	2011–2013	Shell Incentive Fund Scholarship
<i>Scholarship</i>	2010 & 2011	Xerox Corporation Scholarship
<i>Scholarship</i>	2010 & 2011	Intel Academic Award
<i>Grant</i>	June 18, 2010	Cornell University Unmanned Air Systems Team awarded \$1,000 grant, AUVSI Student Unmanned Aerial Systems Competition
<i>Scholarship</i>	2009–2013	Meinig Family Cornell National Scholars
		• Awarded by Peter Meinig (Past Chairman of the Board of Trustees at Cornell University)

## C E R T I F I C A T I O N S

<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