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
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

2022

34. C. Oses, D. Hicks, M. Esters, R. Friedrich, 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. 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*, MRS Bull. **in press** (2022). **arXiv**: arxiv:2111.11519.

32. 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*, Front. Phys. **10**, 815863 (2022). **DOI**: 10.3389/fphy.2022.815863.

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*, Nat. Commun. **12**, 5747 (2021). **DOI**: 10.1038/s41467-021-25979-5.

    • This paper was selected for Editors' 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.

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 **8**, 217 (2021). **DOI**: 10.1038/s41597-021-00974-z.
    [†] 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.

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.

26. M. J. Mehl, M. Ronquillo, D. Hicks, M. Esters, C. Oses, R. Friedrich, A. Smolyanyuk, E. Gossett, D. Finkenstadt & S. Curtarolo, *Tin-pest problem as a test of density functionals using high-throughput calculations*, Phys. Rev. Mater. **5**, 083608 (2021). **DOI**: 10.1103/PhysRevMaterials.5.083608.

25. M. D. Hossain†, T. Borman†, A. Kumar, X. Chen, A. Khosravani, S. R. Kalidindi, E. A. Paisley, M. Esters, C. Oses, C. Toher, S. Curtarolo, J. M. LeBeau, D. W. Brenner & J.-P. Maria, *Carbon Stoichiometry and Mechanical Properties of High Entropy Carbides*, Acta Mater. **215**, 117051 (2021). **DOI**: 10.1016/j.actamat.2021.117051.
   † 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.
   - 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.

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, *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 Editors' 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.

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 Editors' Choice by Elsevier (2017).

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 Editors' 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.
    - This paper was selected for Editors' Choice by the American Chemical Society (2015).

B O O K   P U B L I C A T I O N S

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.

T A L K S / P R E S E N T A T I O N S

Disorder by design: Applications and modeling of high-entropy ceramics

29. **Invited seminar** for the Department of Materials Science and Engineering at Texas A&M University, College Station, Texas — February 10, 2022.

High-entropy ceramics

28. **Invited seminar** for the Department of Physics at the University of Alabama at Birmingham, Birmingham, Alabama — February 04, 2022.

27. **Invited seminar** for the Department of Mechanical Engineering at Rowan University, Glassboro, NJ — January 27, 2022.

26. **Invited seminar** for the Department of Materials Science and Engineering at Johns Hopkins University, Baltimore, MD — January 04, 2022.

25. **Invited seminar** for the Department of Mechanical Engineering at Texas A&M University, College Station, Texas — February 24, 2021.

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

Data for Materials Development Platforms

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

Entropy and ceramics: A valuable partnership

22. **Invited seminar** for the Department of Materials and Interfaces at the Weizmann Institute of Science, Rehovot, Israel — February 06, 2020.

21. **Invited seminar** for the Sackler Center for Computational Molecular and Materials Science at Tel Aviv University, Tel Aviv, Israel — February 05, 2020.

20. **Invited seminar** for the Department of Materials Engineering at Ben-Gurion University of the Negev, Beer Sheva, Israel — January 29, 2020.

Cloud-oriented computational phase diagrams with AFLOW-CHULL

19. **Contributed talk** for the March Meeting of the American Physical Society, Boston, Massachusetts — March 07, 2019.

18. **Poster presentation** for the Open Databases Integration for Materials Design (OPTiMaDe) Workshop of CECAM (Centre Européen de Calcul Atomique et Moléculaire), Lausanne, Switzerland — June 11, 2018.

Going Off-Stoichiometry: Challenging Traditional Materials Discovery

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

Universal Fragment Descriptors for Predicting Properties of Inorganic Crystals

16. **Contributed talk** for the 13th World Congress in Computational Mechanics (WCCM) of the International Association for Computational Mechanics (IACM), New York City, New York — July 23, 2018.

15. **Contributed talk** for the Mach Conference of the Hopkins Extreme Materials Institute (HEMI), Annapolis, Maryland — April 05, 2018.

14. **Contributed talk** for the Chemistry Department's Third Annual Graduate Research Symposium at Duke University, Durham, North Carolina — October 09, 2017.

13. **Contributed talk** for the March Meeting of the American Physical Society, New Orleans, Louisiana — March 14, 2017.

Advancements in Materials Informatics with AFLOW

12. **Invited seminar** for the Theory Department at the Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — January 18, 2018.

11. **Invited seminar** for the Physics Department at the Humboldt University of Berlin, Berlin, Germany — January 16, 2018.

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

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

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

9. **Invited seminar** for the Condensed Matter Physics Seminar Series at Brigham Young University, Provo, Utah — February 18, 2016.

8. **Contributed talk** for the Mechanical Engineering and Materials Science (MEMS) Department's Graduate Student Seminar Series at Duke University, Durham, North Carolina — September 25, 2015.

7. **Contributed talk** for the March Meeting of the American Physical Society, San Antonio, Texas — March 02, 2015.

Plume Propagation Simulation for Pulsed Laser Deposition

6. **Poster presentation** for the Machine Learning Summer School (MLSS) at the University of Texas at Austin, Austin, Texas — January 12, 2015.

5. **Contributed talk** for the NSF/AAAS/EHR Emerging Researchers National Conference, Washington, D.C. — February 22, 2014.

4. **Poster presentation** for the MRS/ASM/AVS/AReMS Meeting, North Carolina State University, Raleigh, North Carolina — November 15, 2013.

3. **Poster presentation** for the Mechanical Engineering and Materials Science (MEMS) Department's Annual Retreat at Duke University, Durham, North Carolina — August 22, 2013.
   - Best Presentation Award

Synchrotron Radiation Focusing Optics — Capillary Beam Stop Design

2. **Contributed talk** for 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** for the LSAMP Research Symposium at Cornell University, Ithaca, New York — August 07, 2012.

Teaching Experience

Co-Instructor	Spring 2021	ME 555: Applications of Artificial Intelligence in Materials, Duke University Department of Mechanical Engineering and Materials Science

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

- Best Teaching Assistant Award, August 14, 2015

W O R K S H O P S

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 — September 6–10, 2021.
    - "Introduction to Density Functional Theory: VASP" recording: https://youtu.be/_RsQH3TY7kI
    - "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, Charlottesville, Virginia — August 17, 2021.
    - "Thermodynamics: AFLOW-CHULL and AFLOW-CCE" recording: https://youtu.be/cLhOcN1sQ7M

11. **Presenter** for the Machine Learning for Materials Research Bootcamp & Workshop on Machine Learning Quantum Materials of NIST/Moore Foundation/University of Maryland, 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 Texas A&M University, 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_cfHIlpBiA

9. **Session Chair** for the Virtual Spring Meeting Tutorial of the Materials Research Society — April 17, 2021.

8. **Presenter** for the Materials 4.0 Summer School 2020 at the Dresden Center for Computational Materials Science (DCMS), Technische Universität (TU) Dresden — August 18, 2020.
    - "Thermodynamics: AFLOW-CHULL" recording: https://youtu.be/ncm356YNBVc

7. **Presenter** for the Machine Learning for Materials Research Bootcamp & Workshop on Machine Learning Quantum Materials of NIST/Moore Foundation/University of Maryland, 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 Texas A&M University, 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** for the Machine Learning for Materials Research Bootcamp & Workshop on Machine Learning Quantum Materials of NIST/Moore Foundation/University of Maryland, Institute for Bioscience & Biotechnology Research in Gaithersburg, Maryland — August 05, 2019.

4. **Organizer and presenter** at the University of Pennsylvania, Philadelphia, Pennsylvania — May 03, 2019.

3. **Organizer and presenter** at the North Carolina State University, Raleigh, North Carolina — March 12, 2019.

2. **Organizer and presenter** at Carnegie Mellon University, Pittsburgh, Pennsylvania — January 21, 2019.

1. **Presenter** for the Machine Learning for Materials Research Bootcamp & Workshop on Machine Learning Quantum Materials of NIST/Moore Foundation/University of Maryland, Institute for Bioscience & Biotechnology Research in Gaithersburg, Maryland — August 02, 2018.

P R E S S   A N D   N E W S   R E L E A S E S

White House Office of Science & Technology Policy	November 18, 2021	*"Featured Vignette in the November 2021 Materials Genome Initiative Strategic Plan (page 9)"*
	mgi.gov/sites/default/files/documents/MGI-2021-Strategic-Plan.pdf	
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

Publication Award	November 16, 2021	"Hot paper", Publication in Nat. Rev. Mater., Web of Science (Clarivate Analytics)
		• 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
Publication Award	2021	Editors' Highlight, Publication in Nat. Commun., Springer Nature
Publication Award	2018	Editors' Choice, Publication in Comput. Mater. Sci., Elsevier
Publication Award	2017	Editors' 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	Editors' Choice, Publication in Comput. Mater. Sci., Elsevier
Publication Award	2015	Editors' Choice, Publication in Chem. Mater., American Chemical Society
Fellowship	2013–2016	Graduate Research Fellowship, National Science Foundation
Award	August 22, 2013	Best Presentation Award at the MEMS Departmental Retreat, Duke University Department of Mechanical Engineering and Materials Science
Award	March 02, 2013	First Place in Nanoscience and Physics Research Presentation, NSF / AAAS / EHR Emerging Researchers National Conference
Scholarship	2011–2013	Shell Incentive Fund Scholarship

Scholarship	2010 & 2011	Xerox Corporation Scholarship
Scholarship	2010 & 2011	Intel Academic Award
Grant	June 18, 2010	Cornell University Unmanned Air Systems Team awarded $1,000 grant, AUVSI Student Unmanned Aerial Systems Competition
Scholarship	2009–2013	Meinig Family Cornell National Scholars

- Awarded by Peter Meinig (Past Chairman of the Board of Trustees at Cornell University)

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