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

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.
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.
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 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.
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, *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 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 Editor's 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 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.
   - 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.

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.

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) 13th World Congress in Computational Mechanics (WCCM), New York City, New York — July 23, 2018.
15. **Contributed talk** at the Hopkins Extreme Materials Institute Mach Conference, Annapolis, Maryland — April 05, 2018.
14. **Contributed talk** at the Duke University Chemistry Department Third Annual Graduate Research Symposium, Durham, North Carolina — October 09, 2017.
13. **Contributed talk** at the American Physical Society March Meeting, New Orleans, Louisiana — March 14, 2017.

Advancements in Materials Informatics with AFLOW

12. **Invited 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

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

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/_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 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_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 (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 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 — 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

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