# COREY OSES

Materials Science and Engineering, Johns Hopkins University

Work Experience - Education - Journal Publications - Book Publications - Teaching Experience - Workshops - Press and News Releases - Honors and Awards

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Google Scholar user=Za7m4CMAAAAJ · citations: 3445 (YTD 1135) · h-index: 22

#### WORK EXPERIENCE

Assistant Professor 2022-present Johns Hopkins University

Postdoctoral Fellow 2018–2022 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

# 2023

- 38. C. Oses, M. Esters, D. Hicks, S. Divilov, H. Eckert, R. Friedrich, M. J. Mehl, A. Smolyanyuk, X. Campilongo, A. van de Walle, J. Schroers, A. G. Kusne, I. Takeuchi, E. Zurek, M. Buongiorno Nardelli, M. Fornari, Y. Lederer, O. Levy, C. Toher & S. Curtarolo, aflow++: a C++ framework for autonomous materials design, Comput. Mater. Sci. 217, 111889 (2023). DOI: 10.1016/j.commatsci.2022.111889. [PDF]
  - This paper was selected for Editor's Choice by Elsevier (2022).
- 37. M. Esters, C. Oses, S. Divilov, H. Eckert, R. Friedrich, D. Hicks, M. J. Mehl, F. Rose, A. Smolyanyuk, A. Calzolari, X. Campilongo, C. Toher & S. Curtarolo, *aflow.org:* a web ecosystem of databases, software and tools, Comput. Mater. Sci. 216, 111808 (2023). DOI: 10.1016/j.commatsci.2022.111808. [PDF]

#### 2022

- 36. A. Calzolari, C. Oses, C. Toher, M. Esters, X. Campilongo, S. P. Stepanoff, D. E. Wolfe & S. Curtarolo, *Plasmonic high-entropy carbides*, Nat. Commun. 13, 5993 (2022). DOI: 10.1038/s41467-022-33497-1. [PDF]
- 35. X. Wang, D. M. Proserpio, C. Oses, C. Toher, S. Curtarolo & E. Zurek, *The Microscopic Diamond Anvil Cell: Stabilization of Superhard, Superconducting Carbon Allotropes at Ambient Pressure*, Angew. Chem. **61**(32), e202205129 (2022). **DOI:** 10.1002/anie.202205129. [PDF]
- 34. H. J. Kulik, T. Hammerschmidt, J. Schmidt, S. Botti, M. A. L. Marques, M. Boley, M. Scheffler, M. Todorović, P. Rinke, C. Oses, A. Smolyanyuk, S. Curtarolo, A. Tkatchenko, A. P. Bartók, S. Manzhos, M. Ihara, T. Carrington, J. Behler, O. Isayev, M. Veit, A. Grisafi, J. Nigam, M. Ceriotti, K. T. Schütt, J. Westermayr, M. Gastegger, R. J. Maurer, B. Kalita, K. Burke, R. Nagai, R. Akashi, O. Sugino, J. Hermann, F. Noé, S. Pilati, C. Draxl, M. Kuban, S. Rigamonti, M. Scheidgen, M. Esters, D. Hicks, C. Toher, P. V. Balachandran, I. Tamblyn, S. Whitelam, C. Bellinger & L. M. Ghiringhelli, Roadmap on Machine Learning in Electronic Structure, Electron. Struct. 4(2), 023004 (2022). DOI: 10.1088/2516-1075/ac572f. [PDF]

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

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*, MRS Bull. 47, 194–202 (2022). DOI: 10.1557/s43577-022-00281-x. [PDF]

#### 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. [PDF]
  - 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. [PDF]
- 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. 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. [PDF]
- 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. [PDF]
- 27. D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. 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.
- 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. [PDF]
- 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. [PDF]
   † 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. [PDF]

  † 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. [PDF]
- C. Oses, C. Toher & S. Curtarolo, High-entropy ceramics, Nat. Rev. Mater. 5, 295–309 (2020). DOI: 10.1038/s41578-019-0170-8. [PDF]
  - 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. [PDF]
- 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. [PDF]
- 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. [PDF]
- 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. [PDF]
- 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. [PDF]

#### 2018

- 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. [PDF]
- 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. [PDF]

 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, High-entropy high-hardness metal carbides discovered by entropy descriptors, Nat. Commun. 9, 4980 (2018). DOI: 10.1038/s41467-018-07160-7. [PDF]

- † 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. [PDF]
- 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. [PDF]
  - This paper was selected for Editor's Choice by Elsevier (2018).
- 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. [PDF]

## 2017

- 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. [PDF]
- 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. [PDF]
  - This paper was selected for Editor's Choice by Elsevier (2017).
- 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. [PDF]
   † 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. [PDF]
- 6. C. Nyshadham, C. Oses, J. E. Hansen, I. Takeuchi, S. Curtarolo & G. L. W. Hart, A Computational High-Throughput Search for New Ternary Superalloys, Acta Mater. 122, 438–447 (2017). DOI: 10.1016/j.actamat.2016.09.017. [PDF]
- 5. S. Sanvito, C. Oses, J. Xue, A. Tiwari, M. Žic, T. Archer, P. Tozman, M. Venkatesan, J. M. 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. [PDF]

### 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. [PDF]
- 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. [PDF]

#### 2015

- C. E. Calderon, J. J. Plata, C. Toher, C. Oses, O. Levy, M. Fornari, A. Natan, M. J. Mehl, G. L. W. 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. [PDF]
  - This paper was selected for Editor's Choice by Elsevier (2015).
- 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. [PDF]
  - This paper was one of the top 10 most highly downloaded papers for the month of January 2015 by the American Chemical Society (2015).
  - This paper was selected for Editors' 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. **DOI**: 10.1002/9783527802265.ch7. [PDF]

#### 2018

 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. [PDF]

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. W. 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\_63-2. [PDF]

TEACHING EXP	ERIENCE	
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  • Best Teaching Assi	ME 221: Structure and Properties of Solids, Duke University Department of Mechanical Engineering and Materials Science istant Award, August 14, 2015

WORKSHOPS

AFLOW School: Integrated infrastructure for computational materials discovery

Co-Organizers: D. Hicks, C. Toher, M. Esters, R. Friedrich, E. Gossett, A. Smolyanyuk, H. Eckert, S. Divilov, F. Rose, M. J. Brenner & S. Curtarolo

- 16. Organizer and presenter at Johns Hopkins University, Baltimore, Maryland September 21, 2022.
  - "Introduction and AFLOW-ML: Machine Learning" recording: https://youtu.be/Xj5BGuFC9ew
- Presenter for the Machine Learning for Materials Research Bootcamp of the University of Maryland/NIST/MRS, College Park, Maryland — August 11, 2022.
- 14. **Organizer and presenter** at the East African Institute for Fundamental Research, University of Rwanda, Kigali, Rwanda February 21–24, 2022.
- 13. **Organizer and presenter** at the Technische Universität (TU) Dresden and Helmholtz-Zentrum Dresden-Rossendorf September 6–10, 2021.
  - "Introduction to Density Functional Theory and VASP" recording: https://youtu.be/\_RsQH3TY7kI
  - "AFLOW-CHULL: Thermodynamics" recording: https://youtu.be/zcY7gTZIB-Y
  - "AFLOW-POCC: Disorder" recording: https://youtu.be/lcDSYiF4AS4
- 12. Organizer and presenter at the University of Virginia, Charlottesville, Virginia August 17, 2021.
  - "AFLOW-CHULL and AFLOW-CCE: Thermodynamics" recording: https://youtu.be/cLhOcN1sQ7M
- 11. **Presenter** for the Machine Learning for Materials Research Bootcamp of the University of Maryland/NIST, College Park, Maryland July 29, 2021.
  - "AFLOW-ML: Machine Learning" 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 and VASP" recording: <a href="https://youtu.be/KXnJGdVgosA">https://youtu.be/KXnJGdVgosA</a>
  - "AFLOW-CHULL and AFLOW-CCE: Thermodynamics" recording: https://youtu.be/ElaniAcrbhU
  - "AFLOW-POCC: Disorder" recording: https://youtu.be/D\_cfHIlpBiA
- 9. Session Chair for the Virtual Spring Meeting 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.
  - "AFLOW-CHULL: Thermodynamics" recording: https://youtu.be/ncm356YNBVc
- 7. **Presenter** for the Machine Learning for Materials Research Bootcamp & Workshop on Machine Learning Microscopy Data of the University of Maryland / NIST, College Park, Maryland July 23, 2020.
  - "AFLOW-ML: Machine Learning" 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 and VASP" recording: https://youtu.be/ChySAfo2w7g
  - "AFLOW-CHULL: Thermodynamics" recording: https://youtu.be/9Sa8D4inJ5w
  - "AFLOW-POCC: Disorder" recording: https://youtu.be/xr-mU-1ShQQ
- 5. **Presenter** for the Machine Learning for Materials Research Bootcamp & Workshop on Autonomous Materials Research of the University of Maryland/NIST, College Park, 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 the University of Maryland/NIST/Moore Foundation, Institute for Bioscience & Biotechnology Research in Gaithersburg, Maryland August 02, 2018.

### PRESS AND NEWS RELEASES

White House Office	November 18,	"Featured Vignette in the November 2021 Materials Genome Initiative		
of Science &	2021	Strategic Plan (page 9)"		
Technology Policy	mgi.gov/sites/default/files/documents/MGI-2021-Strategic-Plan.pdf			
University of	September 2019	"Scientists predict new forms of superhard carbon"		
Buffalo	• This press release is featured on Phys.org, ScienceDaily, SciTechDaily, and Tribonet.			
	buffalo.edu/ubnow/stories/2019/09/zurek-superhard-carbon.html			
Duke University	November 2018	"Disordered Materials Could Be Hardest, Most Heat-Tolerant Ever"		
Pratt School of	• This press release is featured on AAAS EurekAlert!, Phys.org, ScienceDaily, Science Bulletin, Naaju, NewsBeezer, RemoNews, Tech2, and LongRoom News.			
Engineering				
	pratt.duke.edu/about/news/chaotic-carbides			

MRS Bulletin	August 2017 cambridge.org/core	"Universal fragment descriptor predicts materials properties"  /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/r finds-new-uses-curre	news/2017/06/06/breakthrough-tool-predicts-properties-theoretical-materials-ent-ones/
Duke University Pratt School of Engineering	Engineering.com, International Busi	
	pratt.duke.edu/aboi	ut/news/predicting-magnets
MRS Bulletin	April 2015 doi.org/10.1557/mrs	"Materials fingerprints identified for informatics" s.2015.76
Computational Chemistry Highlights	January 2015	"Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints" s.org/2015/01/materials-cartography-representing-and.html
Duke University Research	January 2015 research.duke.edu/r	"Molecular Tornado"  nolecular-tornado
Duke University Graduate School	October 2014 gradschool.duke.edu fellow	"Competing for NSF Fellowships: Advice from a Current Fellow"  1/professional-development/blog/competing-nsf-fellowships-advice-current-
ERN Conference 2013	February 2013 new.emerging-resear	"2013 Oral and Poster Presentation Award Winners" rchers.org/2013-oral-and-poster-presentation-winners
HONORS AND	AWARDS	
Publication Award	2022	Editor's Choice, Publication in Comput. Mater. Sci., Elsevier
Publication Award	November 16, 2021	"Hot paper", Publication in Nat. Rev. Mater., Web of Science (Clarivate Analytics)
		past two years and received enough citations in July/August 2021 to place it in the s in the academic field of Materials Science
Publication Award	2021	Editors' 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	Top 10 most highly downloaded papers for the month of January 2015, Publication in Chem. Mater., American Chemical Society
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	Fall 2010	Dean's Honor List, Cornell University College of Engineering
Scholarship	<ul><li>2009–2013</li><li>Awarded by Peter</li></ul>	Meinig Family Cornell National Scholars er Meinig (Past Chairman of the Board of Trustees at Cornell University)