

# COREY OSES

Materials Science, Duke University

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

email [corey.oses@duke.edu](mailto:corey.oses@duke.edu)  
phone (W) +1 (919) 684 1553  
website [coreyoses.com](http://coreyoses.com)  
Google Scholar [user=Za7m4CMAAAAJ](https://scholar.google.com/citations?user=Za7m4CMAAAAJ) · citations: 2244 (YTD 861) · h-index: 20

## 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

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. 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](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. 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](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  
• This paper was highlighted as an MGI Vignette in the November 2021 Materials Genome Initiative Strategic Plan by the Subcommittee on the Materials Genome Initiative Committee on Technology of the National Science and Technology Council (November 18, 2021).
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, C. Oses, 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).

## 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                           |
|                    |                       | <ul style="list-style-type: none"> <li>• <a href="#">Best Teaching Assistant Award</a>, August 14, 2015</li> </ul>                               |

## 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

University of Buffalo September 2019 “Scientists predict new forms of superhard carbon”

• This press release is featured on [Phys.org](https://www.phys.org), [ScienceDaily](https://www.sciencedaily.com), [SciTechDaily](https://www.scitechdaily.com), and [Tribonet](https://tribonet.com).  
[buffalo.edu/ubnow/stories/2019/09/zurek-superhard-carbon.html](https://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 Engineering  
 • This press release is featured on [AAAS EurekAlert!](https://www.aaas.org), [Phys.org](https://www.phys.org), [ScienceDaily](https://www.sciencedaily.com), [Science Bulletin](https://www.sciencebulletin.com), [Naaju](https://www.naaju.com), [NewsBeezer](https://www.newsbeezer.com), [RemoNews](https://www.remonews.com), [Tech2](https://www.tech2.com), and [LongRoom News](https://www.longroomnews.com).  
[pratt.duke.edu/about/news/chaotic-carbides](https://pratt.duke.edu/about/news/chaotic-carbides)

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| MRS Bulletin                                | August 2017   | <i>"Universal fragment descriptor predicts materials properties"</i><br><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>  |
| UNC Eshelman School of Pharmacy             | June 2017     | <i>"Breakthrough Tool Predicts Properties of Theoretical Materials, Finds New Uses for Current Ones"</i><br><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> <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>  |
| Duke University Pratt School of Engineering | April 2017    | <i>"Computers Create Recipe for Two New Magnetic Materials"</i><br><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> <a href="http://pratt.duke.edu/about/news/predicting-magnets">pratt.duke.edu/about/news/predicting-magnets</a> |
| MRS Bulletin                                | April 2015    | <i>"Materials fingerprints identified for informatics"</i><br><a href="https://doi.org/10.1557/mrs.2015.76">doi.org/10.1557/mrs.2015.76</a>   |
| Computational Chemistry Highlights          | January 2015  | <i>"Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints"</i><br><ul style="list-style-type: none"> <li>"This paper is a <a href="#">tour de force</a> for computational materials science" — Prof. Aspuru-Guzik.</li> </ul> <a href="http://compchemhighlights.org/2015/01/materials-cartography-representing-and.html">compchemhighlights.org/2015/01/materials-cartography-representing-and.html</a>  |
| Duke University Research                    | January 2015  | <i>"Molecular Tornado"</i><br><a href="http://research.duke.edu/molecular-tornado">research.duke.edu/molecular-tornado</a>  |
| Duke University Graduate School             | October 2014  | <i>"Competing for NSF Fellowships: Advice from a Current Fellow"</i><br><a href="http://gradschool.duke.edu/professional-development/blog/competing-nsf-fellowships-advice-current-fellow">gradschool.duke.edu/professional-development/blog/competing-nsf-fellowships-advice-current-fellow</a>  |
| ERN Conference 2013                         | February 2013 | <i>"2013 Oral and Poster Presentation Award Winners"</i><br><a href="http://new.emerging-researchers.org/2013-oral-and-poster-presentation-winners">new.emerging-researchers.org/2013-oral-and-poster-presentation-winners</a>  |

## HONORS AND AWARDS

|                   |                   |   |
|-------------------|-------------------|---|
| Publication Award | November 18, 2021 | MGI Vignette, <a href="#">Publication in Nat. Commun.</a> , Subcommittee on the Materials Genome Initiative Committee on Technology of the National Science and Technology Council  |
| Publication Award | November 16, 2021 | "Hot paper", <a href="#">Publication in Nat. Rev. Mater.</a> , Web of Science (Clarivate Analytics)<br><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, <a href="#">Publication in Nat. Commun.</a> , Springer Nature   |
| Publication Award | 2018              | Editor's Choice, <a href="#">Publication in Comput. Mater. Sci.</a> , Elsevier  |
| Publication Award | 2017              | Editor's Choice, <a href="#">Publication in Comput. Mater. Sci.</a> , Elsevier  |
| Award             | August 14, 2015   | <a href="#">Best Teaching Assistant Award (ME 221)</a> , Duke University Department of Mechanical Engineering and Materials Science   |
| Publication Award | 2015              | Editor's Choice, <a href="#">Publication in Comput. Mater. Sci.</a> , Elsevier  |
| Publication Award | 2015              | Editor's Choice, <a href="#">Publication in Chem. Mater.</a> , American Chemical Society  |
| Fellowship        | 2013–2016         | Graduate Research Fellowship, National Science Foundation   |
| Award             | August 22, 2013   | <a href="#">Best Presentation Award at the MEMS Departmental Retreat</a> , Duke University Department of Mechanical Engineering and Materials Science   |



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|--------------------|--|--|
| <i>Award</i>       | March 02, 2013   | <a href="#">First Place in Nanoscience and Physics Research Presentation</a> , 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  |
|                    | <ul style="list-style-type: none"> <li>• Awarded by Peter Meinig (Past Chairman of the Board of Trustees at Cornell University)</li> </ul> |  |

## 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  |