Corey Oses

Materials Science and Engineering, Johns Hopkins University

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Google Scholar user=Za7m4CMAAAAJ · citations: 4164 (YTD 642) · h-index: 25

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

Current and Pending Support

Current

5. Title: *High-Entropy Capacitive Energy Storage*
   Duration: 07/01/2023 – 06/30/2024
   Funding Level: $150,000
   Agency: Johns Hopkins University, Discovery Award
   PI: C. Oses; co-PI: S. M. Koohpayeh
4. Title: *AFLUX@JHU: Materials Search-API for the JHU* aflow.org *Data Repositories*
   Duration: 06/05/2023 – 08/13/2023
   Funding Level: $6,000
   Agency: Institute for Data Intensive Engineering and Science, 2023 Summer Student Fellowship
   PI: C. Oses
3. Title: *Accelerated Disordered Materials Discovery for Energy Generation in Space*
   Duration: 06/05/2023 – 08/13/2023
   Funding Level: $18,796; Cost-Share: $10,996
   Agency: Maryland Space Grant Consortium, 2023 Summer Student Internship Program
   PI: C. Oses
2. Title: *High-Entropy Metal-Organic Frameworks for High-Performance Lithium-Sulfur Batteries*
   Duration: 04/01/2023 – 03/31/2024
   Funding Level: $25,000
   Agency: Institute for Data Intensive Engineering and Science, 2023 Seed Funding Initiative
   PI: C. Oses; co-PI: V. S. Thoi
1. Title: *Startup Package*
   Duration: 07/01/2022 – 06/30/2024
   Funding Level: $884,624
   Agency: Johns Hopkins University
   PI: C. Oses

Pending

2. Title: *High-Entropy Glass-Ceramics for Nuclear Waste Immobilization*
   Duration: 09/01/2023 – 08/31/2025
   Funding Level: $500,000
   Agency: Advanced Research Projects Agency-Energy (ARPA-E)
   PI: C. Oses; co-PI: S. M. Koohpayeh
1. Title: *Waste-Heat Powered Hydrogen Production on Mars*
   Duration: 09/01/2023 – 08/31/2024
   Funding Level: $25,000
   Agency: Space@Hopkins, 2023 Seed Funding Program
   PI: C. Oses; co-PI: K. A. Kane & A. G. Bregman

Journal Publications

2023

40. D. E. Wolfe, C. M. DeSalle, C. J. Ryan, R. E. Slapikas, R. T. Sweny, R. J. Crealese, P. A. Kolonin, S. P. Stepanoff, A. Haque, S. Divilov, H. Eckert, C. Oses, M. Esters, D. W. Brenner, W. G. Fahrenholtz, J.-P. Maria, C. Toher, E. Zurek & S. Curtarolo, *Influence of Processing on the Microstructural Evolution and Multiscale Hardness in Titanium Carbonitrides (TiCN) Produced via Field Assisted Sintering Technology*, Materialia **27**, 101682 (2023). **DOI**: 10.1016/j.mtla.2023.101682. [PDF]
39. 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).
38. 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]
37. M. Esters†, A. Smolyanyuk†, C. Oses, D. Hicks, S. Divilov, H. Eckert, X. Campilongo, C. Toher & S. Curtarolo, *QH-POCC: taming tiling entropy in thermal expansion calculations of disordered materials*, Acta Mater. **245**, 118594 (2023). **DOI**: 10.1016/j.actamat.2022.118594. [PDF]
    † contributed equally

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†, 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. [PDF]
    † 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. [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.
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. [PDF]
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. [PDF]
    † 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. [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]
22. 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]
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. [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]

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. [PDF]

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

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. [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).
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. [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

2. 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).
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. [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

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. [PDF]
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. 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]

TALKS / PRESENTATIONS

Success Stories in Computationally–Driven Materials Discovery

37. **Invited seminar** for the OneChemistry Symposium, Johns Hopkins University — April 18, 2023.
36. **Invited seminar** for the Computational Spintronics Group at Trinity College Dublin, Trinity College Dublin, Ireland — February 17, 2023.
35. **Invited seminar** for the Physics Department Colloquium at Johns Hopkins University, Baltimore, Maryland — February 15, 2023.

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

34. **Invited seminar** for the Johns Hopkins University Applied Physics Laboratory, Baltimore, Maryland — March 09, 2023.
33. **Invited seminar** for the Hopkins Extreme Materials Institute at Johns Hopkins University, Baltimore, Maryland — November 01, 2022.
32. **Invited seminar** for the Department of Materials Science and Engineering at Texas A&M University, College Station, Texas — February 10, 2022.

Formation Descriptors for High-Entropy High-Hardness Metal Carbides

31. **Invited talk** for the Machine Learning in Ceramics and Glasses Webinar at the Institute of Materials, Minerals and Mining (IOM3), London, UK — March 29, 2022.

High-entropy ceramics

30. **Invited seminar** for the Department of Materials Science and Engineering at Michigan Technological University, Houghton, Michigan — March 17, 2022.
29. **Invited seminar** for the Department of Materials Science and Engineering at the University of California, Irvine, Irvine, California — March 04, 2022.
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

Instructor	Spring 2023	EN.500.113: Gateway Computing: Python, Johns Hopkins University
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: 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
15. **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: https://youtu.be/KXnJGdVgosA
    - "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

Duke University Pratt School of Engineering October 11, 2022 *"Heat-Proof Chaotic Carbides Could Revolutionize Aerospace Technology"*
pratt.duke.edu/about/news/heat-proof-chaotic-carbides-could-revolutionize-aerospace-technology

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"*
	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

Award	2023	Reviewer of the Year, 2022, npj Computational Materials
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)
	• 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	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	2009–2013	Meinig Family Cornell National Scholars

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