Corey Oses

Materials Science and Engineering, Johns Hopkins University

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

email	corey@jhu.edu
phone	(W) +1 (410) 516 5779
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Google Scholar	user=Za7m4CMAAAAJ · citations: 8571 (YTD 1919) · h-index: 35

Work Experience

Assistant Professor	2022–present	Johns Hopkins University
Postdoctoral Fellow	2018–2022	Duke University
Internship	Summer 2013	Cornell High Energy Synchrotron Source (BioSAXS on F2 and G Beamlines)
Internship	Summer 2012	Cornell High Energy Synchrotron Source (Capillary Optics Group)

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

B.Sc. 2009–2013 Cornell University

Department: Applied and Engineering Physics
Thesis: *Plume Propagation Simulation for Pulsed Laser Deposition*

Journal Publications

2025

48. G. Han†, T. Li†, X. Xu, J. Lee, S. Sequeira, A. Ajith & C. Oses*, *The search for high-entropy fuel-cell catalysts using disorder descriptors*, Nano Futures (2025). **DOI**: 10.1088/2399-1984/ae19b0. [PDF]
    † contributed equally
    * corresponding
47. C. Oses*, T. Li, X. Xu, G. Han, G. Qiu & J. R. Owens, *Beyond the four core effects: revisiting thermoelectrics with a high-entropy design*, Mater. Horiz. **12**, 5946–5956 (2025). **DOI**: 10.1039/D5MH00356C. [PDF]
    * corresponding
46. G. Qiu, T. Li, X. Xu, Y. Liu, M. Niyogi, K. Cariaga & C. Oses*, *High entropy powering green energy: hydrogen, batteries, electronics, and catalysis*, npj Comput. Mater. **11**, 145 (2025). **DOI**: 10.1038/s41524-025-01594-6. [PDF]
    * corresponding

2024

45. T. Gong, G. Qiu, M.-R. He, O. V. Safonova, W.-C. Yang, D. Raciti, C. Oses & A. S. Hall, *Atomic Ordering-Induced Ensemble Variation in Alloys Governs Electrocatalyst On/Off States*, J. Am. Chem. Soc. **147**(1), 510–518 (2024). **DOI**: 10.1021/jacs.4c11753. [PDF]
44. K. S. Vecchio, S. Curtarolo, K. Kaufmann, T. J. Harrington, C. Oses & C. Toher, *Fermi energy engineering of enhanced plasticity in high-entropy carbides*, Acta Mater. **276**, 120117 (2024). **DOI**: 10.1016/j.actamat.2024.120117. [PDF]

43. M. L. Evans, J. Bergsma, A. Merkys, C. W. Andersen, O. B. Andersson, D. Beltrán, E. Blokhin, T. M. Boland, R. Castañeda Balderas, K. Choudhary, A. Díaz Díaz, R. Domínguez García, H. Eckert, K. Eimre, M. E. Fuentes-Montero, A. M. Krajewski, J. J. Mortensen, J. M. Nápoles-Duarte, J. Pietryga, J. Qi, F. d. J. Trejo Carrillo, A. Vaitkus, J. Yu, A. C. Zettel, P. Baptista de Castro, J. Carlsson, T. F. T. Cerqueira, S. Divilov, H. Hajiyani, F. Hanke, K. Jose, C. Oses, J. Riebesell, J. Schmidt, D. Winston, C. Xie, X. Yang, S. Bonella, S. Botti, S. Curtarolo, C. Draxl, L. E. Fuentes Cobas, A. Hospital, Z.-K. Liu, M. A. L. Marques, N. Marzari, A. J. Morris, S. P. Ong, M. Orozco, K. A. Persson, K. S. Thygesen, C. Wolverton, M. Scheidgen, C. Toher, G. J. Conduit, G. Pizzi, S. Gražulis, G.-M. Rignanese & R. Armiento, *Developments and applications of the OPTIMADE API for materials discovery, design, and data exchange*, Digit. Discov. **3**, 1509–1533 (2024). **DOI**: 10.1039/D4DD00039K. [PDF]
42. S. Divilov†, H. Eckert†, D. Hicks†, C. Oses†, C. Toher†, R. Friedrich, M. Esters, M. J. Mehl, A. C. Zettel, Y. Lederer, E. Zurek, J.-P. Maria, D. W. Brenner, X. Campilongo, S. Filipović, W. G. Fahrenholtz, C. J. Ryan, C. M. DeSalle, R. J. Crealese, D. E. Wolfe, A. Calzolari & S. Curtarolo, *Disordered enthalpy-entropy descriptor for high-entropy ceramics discovery*, Nature **625**, 66–73 (2024). **DOI**: 10.1038/s41586-023-06786-y. [PDF]
† contributed equally
41. A. B. Peters, D. Zhang, S. Chen, C. Ott, C. Oses, S. Curtarolo, I. McCue, T. Pollock & S. E. Prameela, *Materials Design for Hypersonics*, Nat. Commun. **15**, 3328 (2024). **DOI**: 10.1038/s41467-024-46753-3. [PDF]
    - This paper was selected for Editors' Highlight by Springer Nature (2024).

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]

Teaching Experience

Instructor	Springs 2023–2025	EN.500.113: *Gateway Computing: Python*, Johns Hopkins University
Instructor	Falls 2023–2024	EN.510.666: *Introduction to Computational Materials Modeling*, 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

Service

Mini Symposium on "Computational Thermodynamics: Energy and Energy Landscape"

Co-Organizers: Z.-K. Liu, J. Deng, T. R. Sinno & R. Wentzcovitch

22. **Co-Organizer and Presenter** at the 2025 SIAM New York-New Jersey-Pennsylvania Section Conference, University Park, PA — October 31–November 2, 2025.

Data-Driven Materials Modeling Workshop

Co-Organizers: B. Bukowski & T. Curk

21. **Organizer and Presenter** at Johns Hopkins University, Baltimore, Maryland — May 29–31, 2024.
    - *Data-Driven Thermodynamic Modeling for Materials Discovery* recording: https://youtu.be/kZj3zQkBAKg

Foundations to Futures: Materials Data and AI

Co-Chairs: D. Audus & F. Sen

20. **Conference Co-Chair** at the Materials Research Data Alliance (MaRDA) 2024 Annual Meeting, Baltimore, Maryland — February 20–22, 2024.

Focus Session: Computational Design, Understanding and Discovery of Novel Materials

Co-Chairs: E. Jankowski, R. Sundararaman & D. Usanmaz

19. **Session Chair** for the March Meeting of the American Physical Society, Minneapolis, Minnesota — March 3–8, 2024.

AI, Data Science — Developing the Role for Sustainable Energy in Hopkins' Expansion and Vision

Co-Chair: P. Clancy

18. **Session Co-Chair** at the ROSEI 2024 Summit, Baltimore, Maryland — January 17, 2024.

AFLOW School: Integrated infrastructure for computational materials discovery

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

17. **Presenter** for the Machine Learning for Materials Research Bootcamp of the University of Maryland/NIST/MRS, College Park, Maryland — August 10, 2023.
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. **Co-Organizer and Presenter** at the East African Institute for Fundamental Research, University of Rwanda, Kigali, Rwanda — February 21–24, 2022.
13. **Co-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. **Co-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. **Co-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. **Co-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. **Co-Organizer and Presenter** at the University of Pennsylvania, Philadelphia, Pennsylvania — May 03, 2019.
3. **Co-Organizer and Presenter** at the North Carolina State University, Raleigh, North Carolina — March 12, 2019.
2. **Co-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	2024	Early-Career Investigator Award in Materials Modelling, International Society of Materials Modeling
Publication Award	2024	Editors' Highlight, Publication in Nat. Commun., Springer Nature
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)