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

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Google Scholar user=Za7m4CMAAAAJ · citations: 6283 (YTD 1364) · h-index: 32

Work Experience

Assistant 2022–present Johns Hopkins University

Professor

Postdoctoral 2018–2022 Duke University

Fellow 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

Discoveru

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

2024

- 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., 1509–1533 (2024). DOI: 10.1039/D4DD00039K. [PDF]
- 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

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]
- 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[†], 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

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

- 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[†], 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]
- 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).
- 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

- 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 Experience

U 1		
Instructor	Springs 2023–2024	EN.500.113: <i>Gateway Computing: Python</i> , Johns Hopkins University
Instructor	Fall 2023	EN.510.666: <i>Introduction to Computational Materials Modeling</i> , 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 • Best Teaching Ass	ME 221: Structure and Properties of Solids, Duke University Department of Mechanical Engineering and Materials Science sistant Award, August 14, 2015

Service

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

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

Engineering

White House November 18, Featured Vignette in the November 2021 Materials Genome Initiative

Office of Science 2021 Strategic Plan (page 9)

& Technology mgi.gov/sites/default/files/documents/MGI-2021-Strategic-Plan.pdf

Policy

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 Pratt School of Engineering	NewsBeezer, Ren	Disordered Materials Could Be Hardest, Most Heat-Tolerant Ever e is featured on AAAS EurekAlert!, Phys.org, ScienceDaily, Science Bulletin, Naaju, noNews, Tech2, and LongRoom News. ut/news/chaotic-carbides		
MRS Bulletin	August 2017	Universal fragment descriptor predicts materials properties		
WIKS Bulletin	O	/journals/mrs-bulletin/news/universal-fragment-descriptor-predicts-materials-		
UNC Eshelman School of	June 2017	Breakthrough Tool Predicts Properties of Theoretical Materials, Finds New Uses for Current Ones		
Pharmacy	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/abo	ut/news/predicting-magnets		
MRS Bulletin	April 2015	Materials fingerprints identified for informatics		
	doi.org/10.1557/mrs.2015.76			
Computational Chemistry Highlights	January 2015 compchemhighlight	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/1	Molecular Tornado molecular-tornado		
Duke University Graduate School	October 2014 gradschool.duke.edu fellow	Competing for NSF Fellowships: Advice from a Current Fellow u/professional-development/blog/competing-nsf-fellowships-advice-current-		
ERN Conference	February 2013	2013 Oral and Poster Presentation Award Winners		
2013	new.emerging-researchers.org/2013-oral-and-poster-presentation-winners			
TT 1 A 1				
Honors and Awards Publication	2024	Editors' Highlight, Publication in Nat. Commun., Springer		
Award	2024	Nature 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)		
	\bullet 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	2018	Editor's Choice, Publication in Comput. Mater. Sci., Elsevier		

Award

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) 	