Corey Oses

Materials Science and Engineering, Johns Hopkins University

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website	coreyoses.com
Google Scholar	user=Za7m4CMAAAAJ · citations: 8571 (YTD 1919) · h-index: 35

Objective

To obtain a graduate degree and perform research relevant to Materials Science and Engineering in order to develop my technical and managerial skills toward academia and make significant contributions to Duke University.

Work Experience and Skills

Proficient Coder	Present	`C++`, `Python`, LaTeX, `MATLAB` & `R`
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)
		Developed software for analyzing proteins with SAXS (small angle X-Ray scattering) measurements (Guinier plots).
Internship	Summer 2012	Cornell High Energy Synchrotron Source (Capillary Optics Group)
		Designed a beam stop assembly to eliminate parasitic X-Ray beams and improve focusing capabilities of the ellipsoidal glass capillary optic.
Office Assistant	Summer 2011	ILR Budget Office, Cornell University
Externship	March 2010	Supreme Court of New York
Math Tutor	Fall 2008	Graduate Record Exam (GRE)
Office Assistant	Summer 2008	SOS Security, LLC in Parsippany, NJ

Education

Ph.D.	2013–2018	Duke University
		GPA: 3.8/4.0 · **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
		GPA: 3.3/4.0 · **Department**: Applied and Engineering Physics **Thesis**: *Plume Propagation Simulation for Pulsed Laser Deposition*
High School Diploma	2005–2009	Bloomfield High School
		GPA: 3.9/4.0 · Graduated fifth in class of 428

Funding

Current

5. **Title**: *Next-Generation Mirrors for Harsh Fusion Environments*
   Duration: 01/01/2026 – 12/31/2026
   Funding Level: $145,000
   Agency: Seaver Institute
   Institution: Johns Hopkins University
   PI: C. Oses
4. **Title**: *From Laboratory to Launchpad: Transition Pathways for Climate Science and Energy IP*
   Duration: 07/01/2025 – 06/30/2026
   Funding Level: $115,000
   Agency: Johns Hopkins University, Nexus Convening Award
   Institutions: Johns Hopkins University Applied Physics Laboratory, Johns Hopkins University, and Johns Hopkins Carey Business School
   PIs: A. G. Bregman & C. Oses; **co-PIs**: S. D. Cohen & J. Erlebacher
3. **Title**: *AI-Driven Discovery of High-Entropy H_2 Generators (ADD-H_2)*
   Duration: 07/11/2024 – 12/31/2025
   Funding Level: $1,164,299
   Agency: Johns Hopkins University, SURPASS
   Institutions: Johns Hopkins University and Johns Hopkins University Applied Physics Laboratory
   PIs: C. Oses & A. G. Bregman; **co-PIs**: K. A. Kane, K. K. Rao, V. Leon, A. S. Hall & L. H. Hamilton
2. **Title**: *High-Entropy Glass-Ceramics for Nuclear Waste Immobilization*
   Duration: 09/21/2023 – 09/20/2025
   Funding Level: $500,000
   Agency: Advanced Research Projects Agency-Energy (ARPA-E), Creating Revolutionary Energy And Technology Endeavors (CREATE).
   Institution: Johns Hopkins University
   PI: C. Oses
1. **Title**: *Startup Package*
   Duration: 07/01/2022 – 06/30/2024
   Funding Level: $664,000
   Agency: Johns Hopkins University
   Institution: Johns Hopkins University
   PI: C. Oses

Pending

3. **Title**: *QUENCH$_2$: Quantum Computing of High Entropy Catalysts for Hydrogen Harvesting*
   Duration: 08/01/2025 – 07/31/2028
   Funding Level: $6,468,183; **Cost-Share**: $646,819
   Agency: Advanced Research Projects Agency-Energy (ARPA-E), Quantum Computing for Computational Chemistry (QC^3)
   Institutions: Johns Hopkins University, Johns Hopkins University Applied Physics Laboratory, GTI Energy, and Mattiq
   PI: C. Oses; **co-PIs**: G. Quiroz, M. Bradford & J. Swisher
2. **Title**: *Addressing the Cesium Problem for Negative Hydrogen Ion Sources*
   Duration: 06/01/2025 – 05/31/2027
   Funding Level: $500,000
   Agency: Advanced Research Projects Agency-Energy (ARPA-E), Inspiring Generations of New Innovators to Impact Technologies in Energy 2025 (IGNIITE 2025)
   Institution: Johns Hopkins University
   PI: C. Oses
1. **Title**: *The role of entropy, phase, and disorder in reversible crystalline-amorphous structural transformations*
   Duration: 07/15/2024 – 07/14/2027
   Funding Level: $695,243
   Agency: Department of Energy (DOE), Synthesis and Processing
   Institutions: Johns Hopkins University, University of Connecticut, and University of Illinois at Chicago
   PI: C. Oses; **co-PIs**: S. M. Koohpayeh, A. Dupuy & R. Shahbazian-Yassar

Past

7. **Title**: *Building Trusted Thermodynamic Datasets for Materials Discovery of Metal Iodides*
   Duration: 03/01/2025 – 09/30/2025
   Funding Level: $25,000
   Agency: Data Science and AI Institute, 2025 Trusted Dataset Award
   Institution: Johns Hopkins University
   PI: C. Oses

6. **Title**: *Accelerated Materials Discovery for High-Entropy Hydrogen Fuel Cell Catalysts (HE-FCC)*
   Duration: 06/05/2024 – 08/13/2024
   Funding Level: $6,000
   Agency: Institute for Data Intensive Engineering and Science, 2024 Summer Student Fellowship
   Institution: Johns Hopkins University
   PI: C. Oses
5. **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
   Institutions: Johns Hopkins University and Johns Hopkins University Applied Physics Laboratory
   PI: C. Oses; **co-PIs**: K. A. Kane & A. G. Bregman
4. **Title**: *High-Entropy Capacitive Energy Storage*
   Duration: 07/01/2023 – 06/30/2024
   Funding Level: $150,000
   Agency: Johns Hopkins University, Discovery Award
   Institution: Johns Hopkins University
   PI: C. Oses; **co-PI**: S. M. Koohpayeh
3. **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
   Institution: Johns Hopkins University
   PI: C. Oses
2. **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
   Institution: Johns Hopkins University
   PI: C. Oses
1. **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
   Institution: Johns Hopkins University
   PI: C. Oses; **co-PI**: V. S. Thoi

Journal Publications

2025

48 *The search for high-entropy fuel-cell catalysts using disorder descriptors*
Nano Futures (2025)

Authors: G. Han, T. Li, X. Xu, J. Lee, S. Sequeira, A. Ajith & C. Oses*
† corresponding
Abstract: The transition to a hydrogen economy depends on efficient, affordable catalysts for fuel cells. Platinum—the industry standard for fuel-cell electrodes—is costly and scarce, highlighting the need for practical alternatives. High-entropy alloys offer vast compositional diversity and tunable properties that can mitigate these issues, yet their chemical complexity and configurational disorder have hindered rational discovery. Here, we introduce a data-driven framework that couples machine learning with first-principles disorder descriptors—including the entropy forming ability, disorder enthalpy-entropy descriptor, and electronic-structure similarity metrics to platinum—to predict alloy synthesizability and catalytic performance. These descriptors are applied for the first time in the context of fuel-cell catalyst discovery. The workflow rapidly screens more than 20,000 compositions and identifies several platinum-free candidates that are economically viable, readily scalable, and exhibit promising predicted activity. These results demonstrate that disorder descriptors are reliably predicted by machine learning models and can be effectively integrated into materials-discovery pipelines, accelerating innovation across complex compositional spaces.
DOI: 10.1088/2399-1984/ae19b0

47 *Beyond the four core effects: revisiting thermoelectrics with a high-entropy design*
Mater. Horiz. **12**, 5946–5956 (2025)

Authors: C. Oses*, T. Li, X. Xu, G. Han, G. Qiu & J. R. Owens
† corresponding
Abstract: Low-exergy waste heat, which constitutes the majority of industrial-scale thermal losses, remains largely unrecoverable with conventional technologies. Thermoelectrics offer a solid-state solution for converting this hard-to-access energy into electricity, making them attractive for decentralized power generation and sensor applications. High-entropy materials (HEMs) have gained traction as a strategy for better-performing thermoelectrics, but the mechanisms driving their benefits require further exploration. This article highlights key insights for heat and electronic transport in HEMs. For heat transport, we argue that reduced, and often ultralow, lattice thermal conductivity in HEMs—with respect to ordered counterparts—can be taken for granted, emerging naturally as a fifth core effect of high-entropy systems. While band convergence is often considered beneficial for electronic transport, its impact depends strongly on the electronic structure. We summarize the scenarios where it can be detrimental to thermoelectric performance. These insights motivate strategies that align seamlessly with advancements in artificial intelligence and data-driven approaches, helping accelerate the discovery of next-generation thermoelectric materials.
DOI: 10.1039/D5MH00356C

46 *High entropy powering green energy: hydrogen, batteries, electronics, and catalysis*
npj Comput. Mater. **11**, 145 (2025)

Authors: G. Qiu, T. Li, X. Xu, Y. Liu, M. Niyogi, K. Cariaga & C. Oses*
† corresponding
Abstract: A reformation in energy is underway to replace fossil fuels with renewable sources, driven by the development of new, robust, and multi-functional materials. High-entropy materials (HEMs) have emerged as promising candidates for various green energy applications, having unusual chemistries that give rise to remarkable functionalities. This review examines recent innovations in HEMs, focusing on hydrogen generation/storage, fuel cells, batteries, semiconductors/electronics, and catalysis—where HEMs have demonstrated the ability to outperform state-of-the-art materials. We highlight the role of computational methods, such as density functional theory and machine learning, in accelerating the discovery and optimization of HEMs. The review also presents current challenges and proposes future directions for the field. We emphasize the need for continued integration of modeling, data, and experiments to investigate and leverage the underlying mechanisms of HEMs that are powering progress in sustainable energy.
DOI: 10.1038/s41524-025-01594-6

2024

45 *Atomic Ordering-Induced Ensemble Variation in Alloys Governs Electrocatalyst On/Off States*
J. Am. Chem. Soc. **147**(1), 510–518 (2024)

Authors: T. Gong, G. Qiu, M.-R. He, O. V. Safonova, W.-C. Yang, D. Raciti, C. Oses & A. S. Hall
Abstract: The catalytic behavior of a material is influenced by ensembles—the geometric configuration of atoms on the surface. In conventional material systems, ensemble effects and the electronic structure are coupled because these strategies focus on varying the material composition, making it difficult to understand the role of ensembles in isolation. This study introduces a methodology that separates geometric effects from the electronic structure. To tune the Pd ensemble size on the catalyst surface, we compared the reactivity of structurally different but compositionally identical Pd_3Bi intermetallic and solid solution alloys. Pd_3Bi intermetallics display no reactivity for methanol oxidation (MOR), while their solid solution counterparts show significant reactivity (0.5 mA cm_{Pd}^{-2}). Intermetallics form smaller ensembles (1, 3, 4, and 5 atoms across all low-energy facets), whereas solid solution Pd_3Bi has several facets that support larger Pd ensembles, with an average size of 5.25 atoms and up to 6 atoms. A partially ordered Pd_3Bi (a mixed phase of intermetallic and solid solution) alloy shows intermediate MOR activity (0.1 mA cm_{Pd}^{-2}), confirming that methanol oxidation activity tracks with the average ensemble size. All Pd_3Bi alloys maintained similar electronic structures, as confirmed by X-ray photoelectron spectroscopy (XPS) valence band spectroscopy and X-ray absorption near edge structure (XANES) measurements, indicating that reactivity differences arise from variations in the ensemble size induced by differences in the atomic ordering. Our findings offer an approach for designing materials with controllable active site configurations while maintaining the catalyst's electronic structure, thereby enabling more efficient catalyst design.
DOI: 10.1021/jacs.4c11753

44 *Fermi energy engineering of enhanced plasticity in high-entropy carbides*
Acta Mater. **276**, 120117 (2024)

Authors: K. S. Vecchio, S. Curtarolo, K. Kaufmann, T. J. Harrington, C. Oses & C. Toher
Abstract: Mechanical properties of a range of high-entropy rocksalt carbides are investigated via *ab-initio* modeling and experimental verification. It is found that elastic constants, hardness, and fracture resistance depend on the electronic structure of the system, which is parameterized through two descriptors: the valence electron concentration (VEC) and the integrated density of states from the pseudo-gap energy to the Fermi energy (iDOS(E_{pg}, E_F)). Compositions incorporating more electrons (increasing VEC) shift E_F further above E_{pg}, filling more deformable metal d-derived t_{2g} bonding orbitals. $MoNbTiVWC_5$, $MoNbTaVWC_5$, $CrMoNbVWC_5$, and $CrMoTaVWC_5$, — stabilizing as a single-phase rocksalt solid solution — each have a VEC $\geq$ 9.0, an iDOS(E_{pg}, E_F) $>$ 5.75 states/cell, and a higher electron abundance than any of the rocksalt binary and ternary carbides. The materials approach the ductility range, achieving an attractive combination of fracture resistance (*i.e.* enhanced plasticity) and hardness rarely found in ceramic materials. Entropy, allowing high VEC values to be reached within cubic structures, enables a new path for tailoring mechanical properties.
DOI: 10.1016/j.actamat.2024.120117

43 *Developments and applications of the OPTIMADE API for materials discovery, design, and data exchange*
Digit. Discov. **3**, 1509–1533 (2024)

Authors: 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
Abstract: The Open Databases Integration for Materials Design (OPTIMADE) application programming interface (API) empowers users with holistic access to a growing federation of databases, enhancing the accessibility and discoverability of materials and chemical data. Since the first release of the OPTIMADE specification (v1.0), the API has undergone significant development, leading to the v1.2 release, and has underpinned multiple scientific studies. In this work, we highlight the latest features of the API format, accompanying software tools, and provide an update on the implementation of OPTIMADE in contributing materials databases. We end by providing several use cases that demonstrate the utility of the OPTIMADE API in materials research that continue to drive its ongoing development.
DOI: 10.1039/D4DD00039K

42 *Disordered enthalpy-entropy descriptor for high-entropy ceramics discovery*
Nature **625**, 66–73 (2024)

Authors: 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
† contributed equally
Abstract: The need for improved functionalities in extreme environments is fuelling interest in high-entropy ceramics. Except for the computational discovery of high-entropy carbides, performed with the entropy-forming-ability descriptor4, most innovation has been slowly driven by experimental means1–3. Hence, advancement in the field needs more theoretical contributions. Here we introduce disordered enthalpy– entropy descriptor (DEED), a descriptor that captures the balance between entropy gains and enthalpy costs, allowing the correct classification of functional synthesizability of multicomponent ceramics, regardless of chemistry and structure. To make our calculations possible, we have developed a convolutional algorithm that drastically reduces computational resources. Moreover, DEED guides the experimental discovery of new single-phase high-entropy carbonitrides and borides. This work, integrated into the AFLOW computational ecosystem, provides an array of potential new candidates, ripe for experimental discoveries.
DOI: 10.1038/s41586-023-06786-y

41 *Materials Design for Hypersonics*
Nat. Commun. **15**, 3328 (2024)

Authors: A. B. Peters, D. Zhang, S. Chen, C. Ott, C. Oses, S. Curtarolo, I. McCue, T. Pollock & S. E. Prameela
Abstract: Hypersonic vehicles must withstand extreme conditions during flights that exceed five times the speed of sound. This class of vehicles has the potential to facilitate rapid access to space, bolster defense capabilities, and create a new paradigm for transcontinental earth-to-earth travel. However, the extreme aerothermal environments resulting from high Mach number trajectories create significant challenges for vehicle materials and structures. As hypersonic systems advance, there is a critical need to develop novel materials that are resilient to a combination of thermal and mechanical loads, aggressive oxidizing environments, and rapid heating rates. This work aims to provide a succinct discussion of emerging design strategies for refractory alloys, composites, and ceramics used for hypersonic vehicles. We will highlight key design principles for critical vehicle areas such as primary structures, thermal protection, and propulsion systems; the role of theory and computation in elucidating structure-property-processing relationships; and strategies for advancing laboratory scale materials to flight-ready components such as aerostructures and thermal protection systems.

- This paper was selected for Editors' Highlight by Springer Nature (2024).

DOI: 10.1038/s41467-024-46753-3

2023

40 *Influence of Processing on the Microstructural Evolution and Multiscale Hardness in Titanium Carbonitrides (TiCN) Produced via Field Assisted Sintering Technology*
Materialia **27**, 101682 (2023)

Authors: 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
Abstract: Titanium carbonitride (TiCN) is an advanced, high-performance hard ceramic of great commercial importance that has been widely developed and employed. Nonetheless, it has only been in recent years that binderless titanium carbonitride bulk ceramics have been successfully fabricated using field-assisted sintering technology (FAST). However, the underlying structure-processing-property-performance relationships have yet to be fully evaluated, especially concerning indentation hardness of these materials across a broad range of loads and deformation length scales. In this work we aim to address these fundamental relationships and characterize the multiscale hardness phenomena in detail. It was found that the effects of soak temperature and time directly impacted the sintered microstructure and were reflected in the observed mechanical properties over various loads. Valuable insight into the load-dependence of hardness distributions, sensitivity/correlation with elastoplastic parameters, and multiscale parameterization were developed using micro-/nanoindentation. Particularly, the load-dependent hardness sensitivity and resolvability demonstrate a fundamental tradeoff with respect to the manifested mechanical response influenced by the presence of underlying heterogeneities. These new insights relating the interplay of compositional/microstructural evolution with FAST processing parameters and multiscale hardness are an important step in advancing nextgeneration hard ceramics.
DOI: 10.1016/j.mtla.2023.101682

39 *`aflow++`: a `C++` framework for autonomous materials design*
Comput. Mater. Sci. **217**, 111889 (2023)

Authors: 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
Abstract: The realization of novel technological opportunities given by computational and autonomous materials design requires efficient and effective frameworks. For more than two decades, `aflow++` (Automatic-Flow Framework for Materials Discovery) has provided an interconnected collection of algorithms and workflows to address this challenge. This article contains an overview of the software and some of its most heavily-used functionalities, including algorithmic details, standards, and examples. Key thrusts are highlighted: the calculation of structural, electronic, thermodynamic, and thermomechanical properties in addition to the modeling of complex materials, such as high-entropy ceramics and bulk metallic glasses. The `aflow++` software prioritizes interoperability, minimizing the number of independent parameters and tolerances. It ensures consistency of results across property sets — facilitating machine learning studies. The software also features various validation schemes, offering real-time quality assurance for data generated in a high-throughput fashion. Altogether, these considerations contribute to the development of large and reliable materials databases that can ultimately deliver future materials systems.

- This paper was selected for Editor's Choice by Elsevier (2022).

DOI: 10.1016/j.commatsci.2022.111889

38 *aflow.org: a web ecosystem of databases, software and tools*
Comput. Mater. Sci. **216**, 111808 (2023)

Authors: 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
Abstract: To enable materials databases supporting computational and experimental research, it is critical to develop platforms that both facilitate access to the data and provide the tools used to generate/analyze it — all while considering the diversity of users' experience levels and usage needs. The recently formulated FAIR principles (Findable, Accessible, Interoperable, and Reusable) establish a common framework to aid these efforts. This article describes aflow.org, a web ecosystem developed to provide FAIR-compliant access to the AFLOW databases. Graphical and programmatic retrieval methods are offered, ensuring accessibility for all experience levels and data needs. aflow.org goes beyond data-access by providing applications to important features of the AFLOW software, assisting users in their own calculations without the need to install the entire high-throughput framework. Outreach commitments to provide AFLOW tutorials and materials science education to a global and diverse audiences will also be presented.
DOI: 10.1016/j.commatsci.2022.111808

37 *QH-POCC: taming tiling entropy in thermal expansion calculations of disordered materials*
Acta Mater. **245**, 118594 (2023)

Authors: M. Esters, A. Smolyanyuk, C. Oses, D. Hicks, S. Divilov, H. Eckert, X. Campilongo, C. Toher & S. Curtarolo
Abstract: Disordered materials are attracting considerable attention because of their enhanced properties compared to their ordered analogs, making them particularly suitable for high-temperature applications. The feasibility of incorporating these materials into new devices depends on a variety of thermophysical properties. Among them, thermal expansion is critical to device stability, especially in multi-component systems. Its calculation, however, is quite challenging for materials with substitutional disorder, hindering computational screenings. In this work, we introduce QH-POCC to leverage the local tile-expansion of disorder. This method provides an effective partial partition function to calculate thermomechanical properties of substitutionally disordered compounds in the quasi-harmonic approximation. Two systems, Cu_3Au and Mg_3Cd, are used to validate the methodology by comparing the calculated values of the coefficient of thermal expansion and isobaric heat capacity with experiment, demonstrating that QH-POCC is a promising approach to study thermomechanical properties of disordered systems.
DOI: 10.1016/j.actamat.2022.118594

2022

36 *Plasmonic high-entropy carbides*
Nat. Commun. **13**, 5993 (2022)

Authors: A. Calzolari, C. Oses, C. Toher, M. Esters, X. Campilongo, S. P. Stepanoff, D. E. Wolfe & S. Curtarolo
Abstract: Discovering multifunctional materials with tunable plasmonic properties, capable of surviving harsh environments is critical for advanced optical and telecommunication applications. We chose high-entropy transition-metal carbides because of their exceptional thermal, chemical stability, and mechanical properties. By integrating computational thermodynamic disorder modeling and time-dependent density functional theory characterization, we discovered a crossover energy in the infrared and visible range, corresponding to a metal-to-dielectric transition, exploitable for plasmonics. It was also found that the optical response of high-entropy carbides can be largely tuned from the near-IR to visible when changing the transition metal components and their concentration. By monitoring the electronic structures, we suggest rules for optimizing optical properties and designing tailored high-entropy ceramics. Experiments performed on the archetype carbide $HfTa4C_5$ yielded plasmonic properties from room temperature to 1500K. Here we propose plasmonic transition-metal high-entropy carbides as a class of multifunctional materials. Their combination of plasmonic activity, high-hardness, and extraordinary thermal stability will result in yet unexplored applications.
DOI: 10.1038/s41467-022-33497-1

35 *The Microscopic Diamond Anvil Cell: Stabilization of Superhard, Superconducting Carbon Allotropes at Ambient Pressure*
Angew. Chem. **61**(32), e202205129 (2022)

Authors: X. Wang, D. M. Proserpio, C. Oses, C. Toher, S. Curtarolo & E. Zurek
Abstract: A metallic covalently bonded carbon allotrope is predicted via first principles calculations. It is composed of an sp^3 carbon framework that acts as a diamond anvil cell by constraining the distance between parallel cis-polyacetylene chains. The distance between these sp^2 carbon atoms renders the phase metallic, and yields two well-nested nearly parallel bands that span the Fermi level. Calculations show that this phase is a conventional superconductor, with the motions of the sp^2 carbons being key contributors to the electron phonon coupling. The sp^3 carbon atoms impart superior mechanical properties, with a predicted Vickers hardness of 48 GPa. This phase, metastable at ambient conditions, could be made via cold compression of graphite to 40 GPa. A family of multifunctional materials with tunable superconducting and mechanical properties could be derived from this phase by varying the sp^2 versus sp^3 carbon content and by doping.
DOI: 10.1002/anie.202205129

34 *Roadmap on Machine Learning in Electronic Structure*
Electron. Struct. **4**(2), 023004 (2022)

Authors: 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
Abstract: In recent years, we have been witnessing a paradigm shift in computational materials science. In fact, traditional methods, mostly developed in the second half of the XXth century, are being complemented, extended, and sometimes even completely replaced by faster, simpler, and often more accurate approaches. The new approaches, that we collectively label by machine learning, have their origins in the fields of informatics and artificial intelligence, but are making rapid inroads in all other branches of science. With this in mind, this Roadmap article, consisting of multiple contributions from experts across the field, discusses the use of machine learning in materials science, and share perspectives on current and future challenges in problems as diverse as the prediction of materials properties, the construction of force-fields, the development of exchange correlation functionals for density-functional theory, the solution of the many-body problem, and more. In spite of the already numerous and exciting success stories, we are just at the beginning of a long path that will reshape materials science for the many challenges of the XXIth century.
DOI: 10.1088/2516-1075/ac572f

33 *Physics in the Machine: Integrating Physical Knowledge in Autonomous Phase-Mapping*
Front. Phys. **10**, 815863 (2022)

Authors: A. G. Kusne, A. McDannald, B. DeCost, C. Oses, C. Toher, S. Curtarolo, A. Mehta & I. Takeuchi
Abstract: Application of artificial intelligence (AI), and more specifically machine learning, to the physical sciences has expanded significantly over the past decades. In particular, science-informed AI or scientific AI has grown from a focus on data analysis to now controlling experiment design, simulation, execution and analysis in closed-loop autonomous systems. The CAMEO (closed-loop autonomous materials exploration and optimization) algorithm employs scientific AI to address two tasks: learning a material system's composition-structure relationship and identifying materials compositions with optimal functional properties. By integrating these, accelerated materials screening across compositional phase diagrams was demonstrated, resulting in the discovery of a best-in-class phase change memory material. Key to this success is the ability to guide subsequent measurements to maximize knowledge of the composition-structure relationship, or phase map. In this work we investigate the benefits of incorporating varying levels of prior physical knowledge into CAMEO's autonomous phase-mapping. This includes the use of *ab-initio* phase boundary data from the AFLOW repositories, which has been shown to optimize CAMEO's search when used as a prior.
DOI: 10.3389/fphy.2022.815863

32 *High-entropy ceramics: Propelling applications through disorder*
MRS Bull. **47**, 194–202 (2022)

Authors: C. Toher, C. Oses, M. Esters, D. Hicks, G. N. Kotsonis, C. M. Rost, D. W. Brenner, J.-P. Maria & S. Curtarolo
Abstract: Disorder enhances desired properties, as well as creating new avenues for synthesizing materials. For instance, hardness and yield stress are improved by solid-solution strengthening, a result of distortions and atomic size mismatches. Thermo-chemical stability is increased by the preference of chemically disordered mixtures for high-symmetry super-lattices. Vibrational thermal conductivity is decreased by force-constant disorder without sacrificing mechanical strength and stiffness. Thus, high-entropy ceramics propel a wide range of applications: from wear resistant coatings and thermal and environmental barriers to catalysts, batteries, thermoelectrics and nuclear energy management. Here, we discuss recent progress of the field, with a particular emphasis on disorder-enhanced properties and applications.
DOI: 10.1557/s43577-022-00281-x

2021

31 *Settling the matter of the role of vibrations in the stability of high-entropy carbides*
Nat. Commun. **12**, 5747 (2021)

Authors: M. Esters, C. Oses, D. Hicks, M. J. Mehl, M. Jahnátek, M. D. Hossain, J.-P. Maria, D. W. Brenner, C. Toher & S. Curtarolo
Abstract: High-entropy ceramics are attracting significant interest due to their exceptional chemical stability and physical properties. While configurational entropy descriptors have been successfully implemented to predict their formation and even to discover new materials, the contribution of vibrations to their stability has been contentious. This work unravels the issue by computationally integrating disorder parameterization, phonon modeling, and thermodynamic characterization. Three recently synthesized carbides are used as a testbed: (HfNbTaTiV)C, (HfNbTaTiW)C, and (HfNbTaTiZr)C. It is found that vibrational contributions should not be neglected when precursors or decomposition products have different nearest-neighbor environments from the high-entropy carbide.

- This paper was selected for Editors' Highlight by Springer Nature (2021).

DOI: 10.1038/s41467-021-25979-5

30 *Entropy Landscaping of High-Entropy Carbides*
Adv. Mater. **33**(42), 2102904 (2021)

Authors: 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
Abstract: The entropy landscape of high-entropy carbides can be used to understand and predict their structure, properties, and stability. Using first principles calculations, we analyze the individual and temperature-dependent contributions of vibrational, electronic, and configurational entropies, and compare them qualitatively to the enthalpies of mixing. As an experimental complement, high-entropy carbide thin films were synthesized with high power impulse magnetron sputtering to assess structure and properties. All compositions could be stabilized in the single-phase state despite finite positive, and in some cases substantial, enthalpies of mixing. Density functional theory calculations reveal that configurational entropy dominates the free energy landscape and compensates for the enthalpic penalty, whereas the vibrational and electronic entropies offer negligible contributions. Our calculations predict that in many compositions, the single-phase state becomes stable at extremely high temperatures ($>$ 3000 K). Consequently, rapid quenching rates are needed to preserve solubility at room temperature and facilitate physical characterization. Physical vapor deposition provides this experimental validation opportunity. The computation/experimental data set generated in this work identifies "valence electron concentration" (VEC) as an effective descriptor to predict structural and thermodynamic properties of multicomponent carbides and educate new formulation selections.
DOI: 10.1002/adma.202102904

29 *OPTIMADE: an API for exchanging materials data*
Sci. Data **8**, 217 (2021)

Authors: 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
† contributed equally
Abstract: The Open Databases Integration for Materials Design (OPTIMADE) consortium has designed a universal application programming interface (API) to make materials databases accessible and interoperable. We outline the first stable release of the specification, v1.0, which is already supported by many leading databases and several software packages. We illustrate the advantages of the OPTIMADE API through worked examples on each of the public materials databases that support the full API specification.
DOI: 10.1038/s41597-021-00974-z

28 *Automated coordination corrected enthalpies with AFLOW-CCE*
Phys. Rev. Mater. **5**, 043803 (2021)

Authors: R. Friedrich, M. Esters, C. Oses, S. Ki, M. J. Brenner, D. Hicks, M. J. Mehl, C. Toher & S. Curtarolo
Abstract: The computational design of polar materials poses a critical challenge to thermodynamic modeling since density functional theory yields inaccurate predictions of their formation enthalpies. Progress requires leveraging physically insightful correction methods. The recently introduced coordination corrected enthalpies (CCE) method delivers accurate formation enthalpies with mean absolute errors close to room temperature thermal energy, *i.e.* $\approx$ 25 meV/atom. The CCE scheme, depending on the number of cation-anion bonds and oxidation state of the cation, requires an automated analysis of the system to determine and apply the correction. Here, we present AFLOW-CCE — our implementation of CCE into the AFLOW framework for computational materials design. It features a command line tool, a web interface and a Python environment. The workflow includes a structural analysis, automatically determines oxidation numbers, and accounts for temperature effects by parametrizing vibrational contributions to the formation enthalpy per bond.
DOI: 10.1103/PhysRevMaterials.5.043803

27 *The AFLOW Library of Crystallographic Prototypes: Part 3*
Comput. Mater. Sci. **199**, 110450 (2021)

Authors: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher & S. Curtarolo
Abstract: The *AFLOW Library of Crystallographic Prototypes* has been extended to include a total of 1,100 common crystal structural prototypes (510 new ones with Part 3), comprising all of the inorganic crystal structures defined in the seven-volume *Strukturbericht* series published in Germany from 1937 through 1943. We cover a history of the *Strukturbericht* designation system, the evolution of the system over time, and the first comprehensive index of inorganic *Strukturbericht* designations ever published.
DOI: 10.1016/j.commatsci.2021.110450

26 *Tin-pest problem as a test of density functionals using high-throughput calculations*
Phys. Rev. Mater. **5**, 083608 (2021)

Authors: M. J. Mehl, M. Ronquillo, D. Hicks, M. Esters, C. Oses, R. Friedrich, A. Smolyanyuk, E. Gossett, D. Finkenstadt & S. Curtarolo
Abstract: At ambient pressure tin transforms from its ground-state semi-metal α-Sn (diamond structure) phase to the compact metallic β-Sn phase at 13°C (286K). There may be a further transition to the simple hexagonal γ-Sn above 450K. These relatively low transition temperatures are due to the small energy differences between the structures, ≈ 20 meV/atom between α- and β-Sn. This makes tin an exceptionally sensitive test of the accuracy of density functionals and computational methods. Here we use the high-throughput Automatic-FLOW (AFLOW) method to study the energetics of tin in multiple structures using a variety of density functionals. We look at the successes and deficiencies of each functional. As no functional is completely satisfactory, we look Hubbard U corrections and show that the Coulomb interaction can be chosen to predict the correct phase transition temperature. We also discuss the necessity of testing high-throughput calculations for convergence for systems with small energy differences.
DOI: 10.1103/PhysRevMaterials.5.083608

25 *Carbon Stoichiometry and Mechanical Properties of High Entropy Carbides*
Acta Mater. **215**, 117051 (2021)

Authors: 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
Abstract: The search for new materials via compositional exploration has recently led to the discovery of entropy stabilized and high entropy ceramics. The chemical diversity in the cation sublattice of high entropy ceramics has led to many enhanced properties and applications such as reversible energy storage, low temperature water splitting, amorphous-like thermal transport in crystalline solids and enhanced mechanical properties. This work describes the synthesis and mechanical properties of high entropy (HfNbTaTiZr)C_x thin films as a function of carbon content. The nature of the bonding and microstructure evolves as the material transforms from metallic to ceramic to nanocomposite with variations in the quantity and types of carbon, yielding large variations in the film hardness. Through multiple characterization techniques and first principles investigations, we separate the roles of microstructure and bonding characteristics in the mechanical property development of (HfNbTaTiZr)C_x thin films. This study presents a strategy to establish the bonding, structure, and property relationships in chemically disordered high entropy ceramics, largely based on the relative populations of filled or empty antibonding states for which there are new abilities to do so in high configurational entropy systems that exhibit high solubility of diverse cations while retaining rocksalt structure.
DOI: 10.1016/j.actamat.2021.117051

2020

24 *On-the-fly Closed-loop Autonomous Materials Discovery via Bayesian Active Learning*
Nat. Commun. **11**, 5966 (2020)

Authors: 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
Abstract: The search for advanced materials is hindered by the vast search space of compositions and the exceedingly complex synthesis-processes-structure-property landscape. We demonstrate autonomous research methodology (*i.e.* autonomous hypothesis definition and evaluation) that can place complex, advanced materials in reach, allowing scientists to fail smarter, learn faster, and spend less resources in their studies, while simultaneously improving trust in scientific results and machine learning tools. Additionally, robot science enables science- over-the-network, reducing the economic impact of scientists being separated from their labs. The real-time closed-loop, autonomous system for materials exploration and optimization (CAMEO) is used at the synchrotron beamline to accelerate the fundamentally interconnected tasks of rapid phase mapping and advanced-materials discovery, with each cycle taking seconds to minutes, resulting in the discovery of a novel nanocomposite phase-change memory material.
DOI: 10.1038/s41467-020-19597-w

23 *Discovery of novel high-entropy ceramics via machine learning*
npj Comput. Mater. **6**, 42 (2020)

Authors: K. Kaufmann, D. Maryanovsky, W. M. Mellor, C. Zhu, A. S. Rosengarten, T. J. Harrington, C. Oses, C. Toher, S. Curtarolo & K. S. Vecchio
Abstract: While high-entropy materials are attracting considerable interest due to a combination of useful properties and promising applications, predicting their formation remains a hindrance for rational discovery of new systems. Experimental approaches are based on physical intuition and/or expensive trial and error strategies. Most computational methods rely on the availability of sufficient experimental data and computational power. Machine learning (ML) applied to materials science can accelerate development and reduce costs. In this article, we propose a ML method leveraging thermodynamic and compositional attributes of a given material for predicting the synthesizability (*i.e.* entropy-forming-ability) of disordered metal carbides. The relative importance of the thermodynamic and compositional features for the predictions are then explored. The approach's suitability is demonstrated by comparing values calculated with density functional theory to ML predictions. Finally, the model is employed to predict the entropy-forming-ability of 70 new compositions; several predictions are validated by additional density functional theory calculations and experimental synthesis, corroborating the effectiveness in exploring vast compositional spaces in a high-throughput manner. Importantly, seven compositions are selected specifically because they contain all three of the Group VI elements (Cr, Mo, and W), which do not form room temperature stable rock-salt monocarbides. Incorporating the Group VI elements into the rock-salt structure provides further opportunity for tuning the electronic structure and potentially material performance.
DOI: 10.1038/s41524-020-0317-6

22 *High-entropy ceramics*
Nat. Rev. Mater. **5**, 295–309 (2020)

Authors: C. Oses, C. Toher & S. Curtarolo
Abstract: Disordered multi-component systems, occupying the mostly uncharted centers of phase diagrams, were proposed in 2004 as innovative materials with promising applications. The idea was to maximize the configurational entropy to stabilize (near) equimolar mixtures and achieve more robust systems, which became known as high-entropy materials. Initial research focused mainly on metal alloys and nitride films. In 2015, entropy stabilization was demonstrated in a mixture of oxides. Other high-entropy disordered ceramics rapidly followed, stimulating the addition of more components to obtain materials expressing a blend of properties, often highly enhanced. The systems were soon proven to be useful in wide-ranging technologies, including thermal barrier coatings, thermoelectrics, catalysts, batteries, and wear-resistant and corrosion-resistant coatings. In this Review, we discuss the current state of the disordered ceramics field by examining the applications and the high-entropy features fueling them, covering both theoretical predictions and experimental results. The influence of entropy is unavoidable and can no longer be ignored. In the space of ceramics, it leads to new materials that, both as bulk and thin-films, will play important roles in technology in the decades to come.

- This paper was highlighted as a "hot paper" by Web of Science (Clarivate Analytics) (November 16, 2021).

DOI: 10.1038/s41578-019-0170-8

2019

21 *Metallic glasses for biodegradable implants*
Acta Mater. **176**, 297–305 (2019)

Authors: D. C. Ford, D. Hicks, C. Oses, C. Toher & S. Curtarolo
Abstract: Metallic glasses are excellent candidates for biomedical implant applications due to their inherent strength and corrosion resistance. Use of metallic glasses in structural applications is limited, however, because bulk dimensions are challenging to achieve. Glass-forming ability (GFA) varies strongly with alloy composition and becomes more difficult to predict as the number of chemical species in a system increases. Here we present a theoretical model — implemented in the AFLOW framework — for predicting GFA based on the competition between crystalline phases, and apply it to biologically relevant binary and ternary systems. Elastic properties are estimated based on the rule of mixtures for alloy systems that are predicted to be bulk glass-formers. Focusing on Ca- and Mg-based systems for use in biodegradable orthopedic support applications, we suggest alloys in the AgCaMg and AgMgZn families for further study; and alloys based on the compositions: $Ag_{0.33}Mg_{0.67}$, $Cu_{0.5}Mg_{0.5}$, $Cu_{0.37}Mg_{0.63}$ and $Cu_{0.25}Mg_{0.5}Zn_{0.25}$.
DOI: 10.1016/j.actamat.2019.07.008

20 *Predicting Superhard Materials via a Machine Learning Informed Evolutionary Structure Search*
npj Comput. Mater. **5**, 89 (2019)

Authors: P. Avery, X. Wang, C. Oses, E. Gossett, D. M. Proserpio, C. Toher, S. Curtarolo & E. Zurek
Abstract: Good agreement was found between experimental Vickers hardnesses, H_V, of a wide range of materials and those calculated by three macroscopic hardness models that employ the shear and/or bulk moduli obtained from: (i) first principles via AFLOW-AEL (AFLOW Automatic Elastic Library), and (ii) a machine learning (ML) model trained on materials within the AFLOW repository. Because H_VML values can be quickly estimated, they can be used in conjunction with an evolutionary search to predict stable, superhard materials. This methodology is implemented in the XTALOPT evolutionary algorithm. Each crystal is minimized to the nearest local minimum, and its Vickers hardness is computed via a linear relationship with the shear modulus discovered by Teter. Both the energy/enthalpy and $H^{ML}_{V,Teter}$ are employed to determine a structure's fitness. This implementation is applied towards the carbon system, and 43 new superhard phases are found. A topological analysis reveals that phases estimated to be slightly harder than diamond contain a substantial fraction of diamond and/or lonsdaleite.
DOI: 10.1038/s41524-019-0226-8

19 *Unavoidable disorder and entropy in multi-component systems*
npj Comput. Mater. **5**, 69 (2019)

Authors: C. Toher, C. Oses, D. Hicks & S. Curtarolo
Abstract: The need for improved functionalities is driving the search for more complicated multi-component materials. The competition between enthalpy and entropy is unveiled by statistical analysis of big-data repositories. A threshold in the number of species is found. Beyond that, enthalpy can be neglected, and disorder — complete or partial — is unavoidable.
DOI: 10.1038/s41524-019-0206-z

18 *Coordination corrected ab initio formation enthalpies*
npj Comput. Mater. **5**, 59 (2019)

Authors: R. Friedrich, D. Usanmaz, C. Oses, A. R. Supka, M. Fornari, M. Buongiorno Nardelli, C. Toher & S. Curtarolo
Abstract: The correct calculation of formation enthalpy is one of the enablers of *ab-initio* computational materials design. For several classes of systems (*e.g.* oxides) standard density functional theory produces incorrect values. Here we propose the "coordinationcorrected-enthalpies" method (CCE), based on the number of nearest neighbor cation-anion bonds, and also capable of correcting relative stability of polymorphs. The approach uses calculations employing the PBE, LDA and SCAN exchange correlation functionals, in conjunction with a quasiharmonic Debye model to treat zero-point vibrational and thermal effects. The benchmark, performed on binary and ternary oxides, shows very accurate room temperature results for all functionals, with the smallest mean absolute error of 27 meV/atom obtained with SCAN. The zero-point vibrational and thermal contributions to the formation enthalpies are small and with different signs — largely cancelling each other.
DOI: 10.1038/s41524-019-0192-1

17 *AFLOW-QHA3P: Robust and automated method to compute thermodynamic properties of solids*
Phys. Rev. Mater. **3**, 073801 (2019)

Authors: P. Nath, D. Usanmaz, D. Hicks, C. Oses, M. Fornari, M. Buongiorno Nardelli, C. Toher & S. Curtarolo
Abstract: Accelerating the calculations of finite-temperature thermodynamic properties is a major challenge for rational materials design. Reliable methods can be quite expensive, limiting their applicability in autonomous high-throughput workflows. Here, the three-phonon quasi-harmonic approximation (QHA) method is introduced, requiring only three phonon calculations to obtain a thorough characterization of the material. Leveraging a Taylor expansion of the phonon frequencies around the equilibrium volume, the method efficiently resolves the volumetric thermal expansion coefficient, specific heat at constant pressure, the enthalpy, and bulk modulus. Results from the standard QHA and experiments corroborate the procedure, and additional comparisons are made with the recently developed self-consistent QHA. The three approaches — three-phonon, standard, and self-consistent QHAs — are all included within the open-source framework AFLOW, allowing automated determination of properties with various implementations within the same framework.
DOI: 10.1103/PhysRevMaterials.3.073801

2018

16 *AFLOW-CHULL: Cloud-oriented platform for autonomous phase stability analysis*
J. Chem. Inf. Model. **58**(12), 2477–2490 (2018)

Authors: 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
Abstract: *A priori* prediction of phase stability of materials is a challenging practice, requiring knowledge of all energetically-competing structures at formation conditions. Large materials repositories — housing properties of both experimental and hypothetical compounds — offer a path to prediction through the construction of informatics-based, *ab-initio* phase diagrams. However, limited access to relevant data and software infrastructure has rendered thermodynamic characterizations largely peripheral, despite their continued success in dictating synthesizability. Herein, a new module is presented for autonomous thermodynamic stability analysis implemented within the open-source, *ab-initio* framework AFLOW. Powered by the AFLUX Search-API, AFLOW-CHULL leverages data of more than 1.8 million compounds currently characterized in the AFLOW.org repository and can be employed locally from any UNIX-like computer. The module integrates a range of functionality: the identification of stable phases and equivalent structures, phase coexistence, measures for robust stability, and determination of decomposition reactions. As a proof-of-concept, thorough thermodynamic characterizations have been performed for more than 1,300 binary and ternary systems, enabling the identification of several candidate phases for synthesis based on their relative stability criterion — including 18 promising $C15_b$-type structures and two half-Heuslers. In addition to a full report included herein, an interactive, online web application has been developed showcasing the results of the analysis, and is located at aflow.org/aflow-chull.
DOI: 10.1021/acs.jcim.8b00393

15 *Data-driven design of inorganic materials with the Automatic Flow Framework for Materials Discovery*
MRS Bull. **43**(9), 670–675 (2018)

Authors: C. Oses, C. Toher & S. Curtarolo
Abstract: The expansion of programmatically-accessible materials data has cultivated opportunities for data-driven approaches. Workflows such as the Automatic Flow Framework for Materials Discovery not only manage the generation, storage, and dissemination of materials data, but also leverage the information for thermodynamic formability modeling, such as the prediction of phase diagrams and properties of disordered materials. In combination with standardized parameter sets, the wealth of data is ideal for training machine learning algorithms, which have already been employed for property prediction, descriptor development, design rule discovery, and the identification of candidate functional materials. These methods promise to revolutionize the path to synthesis and, ultimately, transform the practice of traditional materials discovery to one of rational and autonomous materials design.
DOI: 10.1557/mrs.2018.207

14 *High-entropy high-hardness metal carbides discovered by entropy descriptors*
Nat. Commun. **9**, 4980 (2018)

Authors: P. Sarker, T. J. Harrington, C. Toher, C. Oses, M. Samiee, J.-P. Maria, D. W. Brenner, K. S. Vecchio & S. Curtarolo
Abstract: High-entropy materials have attracted considerable interest due to the combination of useful properties and promising applications. Predicting their formation remains the major hindrance to the discovery of new systems. Here we propose a descriptor — entropy forming ability — for addressing synthesizability from first principles. The formalism, based on the energy distribution spectrum of randomized calculations, captures the accessibility of equally-sampled states near the ground state and quantifies configurational disorder capable of stabilizing high-entropy homogeneous phases. The methodology is applied to disordered refractory 5-metal carbides — promising candidates for high-hardness applications. The descriptor correctly predicts the ease with which compositions can be experimentally synthesized as rock-salt high-entropy homogeneous phases, validating the ansatz, and in some cases, going beyond intuition. Several of these materials exhibit hardness up to 50% higher than rule of mixtures estimations. The entropy descriptor method has the potential to accelerate the search for high-entropy systems by rationally combining first principles with experimental synthesis and characterization.
DOI: 10.1038/s41467-018-07160-7

13 *Machine learning modeling of superconducting critical temperature*
npj Comput. Mater. **4**, 29 (2018)

Authors: V. Stanev, C. Oses, A. G. Kusne, E. Rodriguez, J. Paglione, S. Curtarolo & I. Takeuchi
Abstract: Superconductivity has been the focus of enormous research effort since its discovery more than a century ago. Yet, some features of this unique phenomenon remain poorly understood; prime among these is the connection between superconductivity and chemical/structural properties of materials. To bridge the gap, several machine learning methods are developed herein to model the critical temperatures (T_c) of the 12,000+ known superconductors available via the SuperCon database. Materials are first divided into two classes based on their T_c's, above and below 10 K, and a classification model predicting this label is trained. The model uses coarse-grained features based only on the chemical compositions. It shows strong predictive power, with out-of-sample accuracy of about 92%. Separate regression models are developed to predict the values of T_c for cuprate, iron-based, and "low-T_c" compounds. These models also demonstrate good performance, with learned predictors offering important insights into the mechanisms behind superconductivity in different families of materials. To improve the accuracy and interpretability of these models, new features are incorporated using materials data from the AFLOW Online Repositories. Finally, the classification and regression models are combined into a single integrated pipeline and employed to search the entire Inorganic Crystallographic Structure Database (ICSD) for potential new superconductors. We identify about 30 non-cuprate and non-iron-based oxides as candidate materials.
DOI: 10.1038/s41524-018-0085-8

12 *AFLOW-ML: A RESTful API for machine-learning prediction of materials properties*
Comput. Mater. Sci. **152**, 134–145 (2018)

Authors: E. Gossett, C. Toher, C. Oses, O. Isayev, F. Legrain, F. Rose, E. Zurek, J. Carrete, N. Mingo, A. Tropsha & S. Curtarolo
Abstract: Machine learning approaches, enabled by the emergence of comprehensive databases of materials properties, are becoming a fruitful direction for materials analysis. As a result, a plethora of models have been constructed and trained on existing data to predict properties of new systems. These powerful methods allow researchers to target studies only at interesting materials — neglecting the non-synthesizable systems and those without the desired properties — thus reducing the amount of resources spent on expensive computations and/or time-consuming experimental synthesis. However, using these predictive models is not always straightforward. Often, they require a panoply of technical expertise, creating barriers for general users. AFLOW-ML (AFLOW Machine Learning) overcomes the problem by streamlining the use of the machine learning methods developed within the AFLOW consortium. The framework provides an open RESTful API to directly access the continuously updated algorithms, which can be transparently integrated into any workflow to retrieve predictions of electronic, thermal and mechanical properties. These types of interconnected cloud-based applications are envisioned to be capable of further accelerating the adoption of machine learning methods into materials development.

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

DOI: 10.1016/j.commatsci.2018.03.075

11 *AFLOW-SYM: platform for the complete, automatic and self-consistent symmetry analysis of crystals*
Acta Cryst. A **74**, 184–203 (2018)

Authors: D. Hicks, C. Oses, E. Gossett, G. Gomez, R. H. Taylor, C. Toher, M. J. Mehl, O. Levy & S. Curtarolo
Abstract: Determination of the symmetry profile of structures is a persistent challenge in materials science. Results often vary amongst standard packages, hindering autonomous materials development by requiring continuous user attention and educated guesses. This article presents a robust procedure for evaluating the complete suite of symmetry properties, featuring various representations for the point, factor and space groups, site symmetries and Wyckoff positions. The protocol determines a system-specific mapping tolerance that yields symmetry operations entirely commensurate with fundamental crystallographic principles. The self-consistent tolerance characterizes the effective spatial resolution of the reported atomic positions. The approach is compared with the most used programs and is successfully validated against the space-group information provided for over 54,000 entries in the Inorganic Crystal Structure Database (ICSD). Subsequently, a complete symmetry analysis is applied to all 1.7+ million entries of the AFLOW data repository. The AFLOW-SYM package has been implemented in, and made available for, public use through the automated *ab initio* framework AFLOW.
DOI: 10.1107/S2053273318003066

2017

10 *The structure and composition statistics of 6A binary and ternary structures*
Inorg. Chem. **57**(2), 653–667 (2017)

Authors: A. Hever, C. Oses, S. Curtarolo, O. Levy & A. Natan
Abstract: The fundamental principles underlying the arrangement of the elements into solid compounds with an enormous variety of crystal structures are still largely unknown. This study presents a general overview of the structure types appearing in an important subset of the solid compounds, *i.e.*, binary and ternary compounds of the 6A column oxides, sulfides and selenides. It contains an analysis of these compounds, including the prevalence of various structure types, their symmetry properties, compositions, stoichiometries and unit cell sizes. It is found that these compound families include preferred stoichiometries and structure types, some of which have highly specific atomic compositions that may reflect both their specific chemistry and research bias in the available empirical data.
DOI: 10.1021/acs.inorgchem.7b02462

9 *AFLUX: The LUX materials search API for the AFLOW data repositories*
Comput. Mater. Sci. **137**, 362–370 (2017)

Authors: F. Rose, C. Toher, E. Gossett, C. Oses, M. Buongiorno Nardelli, M. Fornari & S. Curtarolo
Abstract: Automated computational materials science frameworks rapidly generate large quantities of materials data for accelerated materials design. In order to take advantage of these large databases, users should have the ability to efficiently search and extract the desired data. Therefore, we have extended the data oriented AFLOW-repository Application-Program-Interface (API) (Comput. Mater. Sci. **93**, 178 (2014)) to enable programmatic access to search queries. A Uniform Resource Identifier (URI)-based search API is proposed for the construction of complex queries for remote creation and retrieval of customized data sets. It is expected that the new language AFLUX, from Automatic Flow of LUX (light), will enable remote search operations on the AFLOW set of computational materials science data repositories. In addition, AFLUX facilitates the verification and validation of the data in the AFLOW repositories.

- This paper was selected for Editor's Choice by Elsevier (2017).

DOI: 10.1016/j.commatsci.2017.04.036

8 *Universal Fragment Descriptors for Predicting Properties of Inorganic Crystals*
Nat. Commun. **8**, 15679 (2017)

Authors: O. Isayev, C. Oses†, C. Toher, E. Gossett, S. Curtarolo & A. Tropsha
† contributed equally
Abstract: Historically, materials discovery is driven by a laborious trial-and-error process. The growth of materials databases and emerging informatics approaches finally offer the opportunity to transform this practice into data- and knowledge-driven rational design-accelerating discovery of novel materials exhibiting desired properties. By using data from the AFLOW repository for high-throughput ab-initio calculations, we have generated Quantitative Materials Structure-Property Relationship (QMSPR) models to predict three critical material properties, namely the metal / insulator classification, Fermi energy, and band gap energy. The prediction accuracy obtained with these QMSPR models approaches training data for virtually any stoichiometric inorganic crystalline material. We attribute the success and universality of these models to the construction of new material descriptors-referred to as the universal property-labeled material fragments (PLMF). This representation affords straightforward model interpretation in terms of simple heuristic design rules that could guide rational materials design. This proof-of-concept study demonstrates the power of materials informatics to dramatically accelerate the search for new materials.
DOI: 10.1038/ncomms15679

7 *Combining the AFLOW GIBBS and elastic libraries to efficiently and robustly screening thermomechanical properties of solids*
Phys. Rev. Mater. **1**, 015401 (2017)

Authors: 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
Abstract: Thorough characterization of the thermomechanical properties of materials requires difficult and time-consuming experiments. This severely limits the availability of data and is one of the main obstacles for the development of effective accelerated materials design strategies. The rapid screening of new potential systems requires highly integrated, sophisticated, and robust computational approaches. We tackled the challenge by developing an automated, integrated workflow with robust error-correction within the AFLOW framework which combines the newly developed "Automatic Elasticity Library" with the previously implemented GIBBS method. The first extracts the mechanical properties from automatic self-consistent stress-strain calculations, while the latter employs those mechanical properties to evaluate the thermodynamics within the Debye model. The new thermoelastic library is benchmarked against a set of 74 experimentally characterized systems to pinpoint a robust computational methodology for the evaluation of bulk and shear moduli, Poisson ratios, Debye temperatures, Grüneisen parameters, and thermal conductivities of a wide variety of materials. The effect of different choices of equations of state and exchange-correlation functionals is examined and the optimum combination of properties for the Leibfried-Schlömann prediction of thermal conductivity is identified, leading to improved agreement with experimental results than the GIBBS-only approach. The framework has been applied to the AFLOW.org data repositories to compute the thermoelastic properties of over 3500 unique materials. The results are now available online by using an expanded version of the REST-API described in the Appendix.
DOI: 10.1103/PhysRevMaterials.1.015401

6 *A Computational High-Throughput Search for New Ternary Superalloys*
Acta Mater. **122**, 438–447 (2017)

Authors: C. Nyshadham, C. Oses, J. E. Hansen, I. Takeuchi, S. Curtarolo & G. L. W. Hart
Abstract: In 2006, a novel cobalt-based superalloy was discovered with mechanical properties better than some conventional nickel-based superalloys. As with conventional superalloys, its high performance arises from the precipitate-hardening effect of a coherent $L1_2$ phase, which is in two-phase equilibrium with the fcc matrix. Inspired by this unexpected discovery of an $L1_2$ ternary phase, we performed a first-principles search through 2224 ternary metallic systems for analogous precipitate-hardening phases of the form $X_3[A_{0.5}, B_{0.5}]$, where X = Ni, Co, or Fe, and [A, B] = Li, Be, Mg, Al, Si, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn Ga, Sr, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn, Sb, Hf, Ta, W, Re, Os, Ir, Pt, Au, Hg, or Tl. We found 102 systems that have a smaller decomposition energy and a lower formation enthalpy than the Co_3(Al, W) superalloy. They have a stable two-phase equilibrium with the host matrix within the concentration range $0 < x < 1$ ($X_3[A_x, B_{1-x}]$) and have a relative lattice mismatch with the host matrix of less than or equal to 5%. These new candidates, narrowed from 2224 systems, suggest possible experimental exploration for identifying new superalloys. Of these 102 systems, 37 are new; they have no reported phase diagrams in standard databases. Based on cost, experimental difficulty, and toxicity, we limit these 37 to a shorter list of six promising candidates of immediate interest. Our calculations are consistent with current experimental literature where data exists.
DOI: 10.1016/j.actamat.2016.09.017

5 *Accelerated Discovery of New Magnets in the Heusler Alloy Family*
Sci. Adv. **3**(4), e1602241 (2017)

Authors: S. Sanvito, C. Oses, J. Xue, A. Tiwari, M. Žic, T. Archer, P. Tozman, M. Venkatesan, J. M. D. Coey & S. Curtarolo
Abstract: Magnetic materials underpin modern technologies, ranging from data storage to energy conversion to contactless sensing. However, the development of a new high-performance magnet is a long and often unpredictable process, and only about two dozen feature in mainstream applications. We describe a systematic pathway to the design of novel magnetic materials, which demonstrates a high throughput and discovery speed. On the basis of an extensive electronic structure library of Heusler alloys containing 236,115 prototypical compounds, we filtered those alloys displaying magnetic order and established whether they can be fabricated at thermodynamical equilibrium. Specifically, we carried out a full stability analysis of intermetallic Heusler alloys made only of transition metals. Among the possible 36,540 prototypes, 248 were thermodynamically stable but only 20 were magnetic. The magnetic ordering temperature, T_C, was estimated by a regression calibrated on the experimental T_C of about 60 known compounds. As a final validation, we attempted the synthesis of a few of the predicted compounds and produced two new magnets: Co_2MnTi, which displays a remarkably high T_C in perfect agreement with the predictions, and Mn_2PtPd, which is an antiferromagnet. Our work paves the way for large-scale design of novel magnetic materials at potentially high speed.
DOI: 10.1126/sciadv.1602241

2016

4 *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)

Authors: A. van Roekeghem, J. Carrete, C. Oses, S. Curtarolo & N. Mingo
Abstract: Using finite-temperature phonon calculations and machine-learning methods, we assess the mechanical stability of about 400 semiconducting oxides and fluorides with cubic perovskite structures at 0, 300, and 1000 K. We find 92 mechanically stable compounds at high temperatures — including 36 not mentioned in the literature so far — for which we calculate the thermal conductivity. We show that the thermal conductivity is generally smaller in fluorides than in oxides, largely due to a lower ionic charge, and describe simple structural descriptors that are correlated with its magnitude. Furthermore, we show that the thermal conductivities of most cubic perovskites decrease more slowly than the usual T^{-1} behavior. Within this set, we also screen for materials exhibiting negative thermal expansion. Finally, we describe a strategy to accelerate the discovery of mechanically stable compounds at high temperatures.
DOI: 10.1103/PhysRevX.6.041061

3 *Modeling Off-Stoichiometry Materials with a High-Throughput Ab-Initio Approach*
Chem. Mater. **28**(18), 6484–6492 (2016)

Authors: K. Yang, C. Oses & S. Curtarolo
Abstract: Predicting material properties of off-stoichiometry systems remains a long-standing and formidable challenge in rational materials design. A proper analysis of such systems by means of a supercell approach requires the exhaustive consideration of all possible superstructures, which can be a time-consuming process. On the contrary, the use of quasirandom approximants, although very computationally effective, implicitly bias the analysis toward disordered states with the lowest site correlations. Here, we propose a novel framework designed specifically to investigate stoichiometrically driven trends of disordered systems (*i.e.*, having partial occupation and/or disorder in the atomic sites). At the heart of the approach is the identification and analysis of unique supercells of a virtually equivalent stoichiometry to the disordered material. We employ Boltzmann statistics to resolve system-wide properties at a high-throughput (HT) level. To maximize efficiency and accessibility, we integrated the method within the automatic HT computational framework AFLOW. As proof of concept, we apply our approach to three systems of interest, a zinc chalcogenide ($ZnS_{1-x}Se_x$), a wide-gap oxide semiconductor ($Mg_xZn_{1-x}O$), and an iron alloy ($Fe_{1-x}Cu_x$), at various stoichiometries. These systems exhibit properties that are highly tunable as a function of composition, characterized by optical bowing and linear ferromagnetic behavior. Not only are these qualities successfully predicted, but additional insight into underlying physical mechanisms is revealed.
DOI: 10.1021/acs.chemmater.6b01449

2015

2 *The AFLOW Standard for High-Throughput Materials Science Calculations*
Comput. Mater. Sci. **108A**, 233–238 (2015)

Authors: 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
Abstract: The Automatic-Flow (AFLOW) standard for the high-throughput construction of materials science electronic structure databases is described. Electronic structure calculations of solid state materials depend on a large number of parameters which must be understood by researchers, and must be reported by originators to ensure reproducibility and enable collaborative database expansion. We therefore describe standard parameter values for k-point grid density, basis set plane wave kinetic energy cut-off, exchange-correlation functionals, pseudopotentials, DFT+U parameters, and convergence criteria used in AFLOW calculations.

- This paper was selected for Editor's Choice by Elsevier (2015).

DOI: 10.1016/j.commatsci.2015.07.019

1 *Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints*
Chem. Mater. **27**(3), 735–743 (2015)

Authors: O. Isayev, D. Fourches, E. N. Muratov, C. Oses, K. M. Rasch, A. Tropsha & S. Curtarolo
Abstract: As the proliferation of high-throughput approaches in materials science is increasing the wealth of data in the field, the gap between accumulated-information and derived-knowledge widens. We address the issue of scientific discovery in materials databases by introducing novel analytical approaches based on structural and electronic materials fingerprints. The framework is employed to *(i)* query large databases of materials using similarity concepts, *(ii)* map the connectivity of materials space (*i.e.*, as a materials cartograms) for rapidly identifying regions with unique organizations / properties, and *(iii)* develop predictive Quantitative Materials Structure-Property Relationship models for guiding materials design. In this study, we test these fingerprints by seeking target material properties. As a quantitative example, we model the critical temperatures of known superconductors. Our novel materials fingerprinting and materials cartography approaches contribute to the emerging field of materials informatics by enabling effective computational tools to analyze, visualize, model, and design new materials.

- 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).

DOI: 10.1021/cm503507h

Book Publications

2019

3 *Automated computation of materials properties*
Materials Informatics: Methods, Tools and Applications, Ch. 7

Authors: C. Toher, C. Oses & S. Curtarolo
Abstract: Materials informatics offers a promising pathway towards rational materials design, replacing the current trial-and-error approach and accelerating the development of new functional materials. Through the use of sophisticated data analysis techniques, underlying property trends can be identified, facilitating the formulation of new design rules. Such methods require large sets of consistently generated, programmatically accessible materials data. Computational materials design frameworks using standardized parameter sets are the ideal tools for producing such data. This work reviews the state-of-the-art in computational materials design, with a focus on these automated *ab-initio* frameworks. Features such as structural prototyping and automated error correction that enable rapid generation of large datasets are discussed, and the way in which integrated workflows can simplify the calculation of complex properties, such as thermal conductivity and mechanical stability, is demonstrated. The organization of large datasets composed of *ab-initio* calculations, and the tools that render them programmatically accessible for use in statistical learning applications, are also described. Finally, recent advances in leveraging existing data to predict novel functional materials, such as entropy stabilized ceramics, bulk metallic glasses, thermoelectrics, superalloys, and magnets, are surveyed.
DOI: 10.1002/9783527802265.ch7

2018

2 *Machine learning and high-throughput approaches to magnetism*
Handbook of Materials Modeling. Volume 2 Applications: Current and Emerging Materials

Authors: S. Sanvito, M. Žic, J. Nelson, T. Archer, C. Oses & S. Curtarolo
Abstract: Magnetic materials have underpinned human civilization for at least one millennium and now find applications in the most diverse technologies, ranging from data storage, to energy production and delivery, to sensing. Such great diversity, associated to the fact that only a limited number of elements can sustain a magnetic order, makes magnetism rare and fascinating. The discovery of a new high-performance magnet is often a complex process, where serendipity plays an important role. Here we present a range of novel approaches to the discovery and design of new magnetic materials, which is rooted in high-throughput electronic structure theory and machine learning models. Such combination of methods has already demonstrated the ability of discovering ferromagnets with high Curie temperature at an unprecedented speed.
DOI: 10.1007/978-3-319-50257-1_108-1

1 *The AFLOW Fleet for Materials Discovery*
Handbook of Materials Modeling. Volume 1 Methods: Theory and Modeling

Authors: 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
Abstract: The traditional paradigm for materials discovery has been recently expanded to incorporate substantial data driven research. With the intent to accelerate the development and the deployment of new technologies, the AFLOW Fleet for computational materials design automates high-throughput first principles calculations, and provides tools for data verification and dissemination for a broad community of users. AFLOW incorporates different computational modules to robustly determine thermodynamic stability, electronic band structures, vibrational dispersions, thermo-mechanical properties and more. The AFLOW data repository is publicly accessible online at aflow.org, with more than 1.7 million materials entries and a panoply of queryable computed properties. Tools to programmatically search and process the data, as well as to perform online machine learning predictions, are also available.
DOI: 10.1007/978-3-319-42913-7_63-2

Talks/Presentations

From Data to Discovery: Active Learning Unlocks Complex Ceramic Design Spaces

63. **Invited talk** for the Mini Symposium on "Computational Thermodynamics: Energy and Energy Landscape" at the 2025 SIAM New York-New Jersey-Pennsylvania Section Conference, University Park, PA — November 02, 2025.

AI Materials Discovery for Nuclear Waste and Spent Fuel Immobilization

62. **Invited talk** for the 2025 Annual Fission Workshop of the Advanced Research Projects Agency-Energy (ARPA-E), Arlington, VA — October 02, 2025.

Accelerating Energy Solutions with High-Entropy Materials: Leveraging Disorder, Computation, and AI

61. **Invited talk** for the The Advanced Materials Show at MS&T25 Technical Meeting and Exhibition, Columbus, OH — September 30, 2025.

High-Entropy Alloys and Halides: Expanding the Energy-Materials Space

60. **Invited talk** for the Symposium on "Advances in Refractory High Entropy Alloys and Ceramics" at the MS&T25 Technical Meeting and Exhibition, Columbus, OH — September 30, 2025.

High-Entropy Oxides and Halides: Expanding the Energy-Materials Space

59. **Invited talk** for the Artificial Intelligence for Materials Science (AIMS) Workshop at the National Institute of Standards and Technology (NIST), Rockville, MD — June 10, 2025.
    - *Artificial Intelligence for Materials Science (AIMS) Workshop* recording: https://www.nist.gov/news-events/events/2025/07/artificial-intelligence-materials-science-aims-workshop

High-Entropy Halides: Expanding the Energy-Materials Space

58. **Invited talk** for the Symposium on "High Entropy and Complex Structure for Electrocatalysis and Other Applications" at the ACS Spring 2025 Meeting & Expo, San Diego, CA — March 25, 2024.
57. **Invited talk** for the Symposium on "Advances in Ceramic Materials and Processing" at the TMS 2025 Annual Meeting & Exhibition, Las Vegas, NV — March 24, 2025.

Metal Iodide Materials for Energy Applications

56. **Invited talk** for the Symposium on "Understanding High Entropy Materials Via Data-Science and Computational Approaches" at the MS&T24 Technical Meeting and Exhibition, Pittsburgh, PA — October 09, 2024.

Success Stories in Computationally–Driven Materials Discovery

55. **Invited seminar** for the Departmental Seminar Series at the Department of Materials Science and Engineering at the University of Connecticut, Storrs, CT — September 27, 2024.
54. **Contributed talk** for the Symposium on "Machine learning assisted materials discovery" at the 11th International Conference on Multiscale Materials Modeling (MMM11), Prague, Czech Republic — September 24, 2024.
53. **Invited seminar** for the Departmental Seminar Series at the Department of Chemical and Nano Engineering at the University of California, San Diego, San Diego, CA — May 01, 2024.
52. **Invited seminar** for the Materials Science and Engineering Fall Seminar Series at the Rensselaer Polytechnic Institute, Troy, NY — October 18, 2023.
51. **Invited seminar** for the Physics Department Colloquium at Georgetown University, Washington, DC — September 26, 2023.
50. **Invited seminar** for the OneChemistry Symposium, Johns Hopkins University — April 18, 2023.
49. **Invited seminar** for the Computational Spintronics Group, Trinity College Dublin, Ireland — February 17, 2023.
48. **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

47. **Invited talk** for the Symposium on "Advancing Ab-Initio Force Fields with Machine-Learning for Energy Materials" at the International Conference on Computational & Experimental Engineering and Sciences (ICCES 2024), Singapore — August 04, 2024.
46. **Invited seminar** for the Departmental Seminar Series at the University of Michigan, Ann Arbor, MI — March 04, 2024.
45. **Invited seminar** for the Johns Hopkins University Applied Physics Laboratory, Baltimore, Maryland — March 09, 2023.
44. **Invited seminar** for the Hopkins Extreme Materials Institute at Johns Hopkins University, Baltimore, Maryland — November 01, 2022.
43. **Invited seminar** for the Department of Materials Science and Engineering at Texas A&M University, College Station, Texas — February 10, 2022.

Bayesian Optimization of the PhD (and beyond)

42. **Keynote** for the Fifth Annual Research Summit for the University Center of Exemplary Mentoring at Duke University, Durham, NC — February 29, 2024.

Computational Materials Science

41. **Invited seminar** for the PARADIM Summer School, Johns Hopkins University — August 02, 2023.

Formation Descriptors for High-Entropy High-Hardness Metal Carbides

40. **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

39. **Invited seminar** for the Department of Materials Science and Engineering at Michigan Technological University, Houghton, Michigan — March 17, 2022.
38. **Invited seminar** for the Department of Materials Science and Engineering at the University of California, Irvine, Irvine, CA — March 04, 2022.
37. **Invited seminar** for the Department of Physics at the University of Alabama at Birmingham, Birmingham, Alabama — February 04, 2022.
36. **Invited seminar** for the Department of Mechanical Engineering at Rowan University, Glassboro, NJ — January 27, 2022.
35. **Invited seminar** for the Department of Materials Science and Engineering at Johns Hopkins University, Baltimore, MD — January 04, 2022.
34. **Invited seminar** for the Department of Mechanical Engineering at Texas A&M University, College Station, Texas — February 24, 2021.
33. **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

32. **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

31. **Invited seminar** for the Department of Materials and Interfaces at the Weizmann Institute of Science, Rehovot, Israel — February 06, 2020.
30. **Invited seminar** for the Sackler Center for Computational Molecular and Materials Science at Tel Aviv University, Tel Aviv, Israel — February 05, 2020.
29. **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

28. **Contributed talk** for the March Meeting of the American Physical Society, Boston, Massachusetts — March 07, 2019.
27. **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

26. **Invited seminar** for the Center for Computational Materials Science at the Naval Research Laboratory, Washington, D.C. — January 09, 2019.

AFLOW-CHULL: Cloud-oriented platform for autonomous phase stability analysis

25. **Contributed talk** for the SHPE National Conference, Cleveland, Ohio — November 09, 2018.
    - Presentation Finalist at the Engineering Science Symposium

Machine learning, phase stability, and disorder with the Automatic Flow Framework for Materials Discovery

24. **PhD defense** for the Ph.D. Thesis Defense at Duke University, Durham, North Carolina — October 31, 2018.
    - Passed thesis defense
23. **PhD preliminary exam** for the Ph.D. Preliminary Exam at Duke University, Durham, North Carolina — June 24, 2016.
    - Passed preliminary examination
22. **PhD qualifying exam** for the Ph.D. Qualifying Exam at Duke University, Durham, North Carolina — August 07, 2014.
    - Passed qualifying examination
    - Subjects: Computational Materials Science, Statistical Mechanics, and Applied Partial Differential Equations and Complex Variables

Universal Fragment Descriptors for Predicting Properties of Inorganic Crystals

21. **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.
20. **Contributed talk** for the Mach Conference of the Hopkins Extreme Materials Institute (HEMI), Annapolis, Maryland — April 05, 2018.
19. **Contributed talk** for the SHPE National Conference, Kansas City, Missouri — November 03, 2017.
    - Presentation Winner at the Engineering Science Symposium
18. **Contributed talk** for the Chemistry Department's Third Annual Graduate Research Symposium at Duke University, Durham, North Carolina — October 09, 2017.
17. **Contributed talk** for the March Meeting of the American Physical Society, New Orleans, Louisiana — March 14, 2017.

Advancements in Materials Informatics with AFLOW

16. **Invited seminar** for the Theory Department at the Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — January 18, 2018.
15. **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

14. **Contributed talk** for the SHPE National Conference, Seattle, Washington — November 04, 2016.
    - Presentation Finalist at the Engineering Science Symposium
13. **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

12. **Invited seminar** for the Condensed Matter Physics Seminar Series at Brigham Young University, Provo, Utah — February 18, 2016.
11. **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.
10. **Contributed talk** for the March Meeting of the American Physical Society, San Antonio, Texas — March 02, 2015.

Plume Propagation Simulation for Pulsed Laser Deposition

9. **Poster presentation** for the Machine Learning Summer School (MLSS) at the University of Texas at Austin, Austin, Texas — January 12, 2015.
8. **Contributed talk** for the NSF/AAAS/EHR Emerging Researchers National Conference, Washington, D.C. — February 22, 2014.
7. **Poster presentation** for the MRS/ASM/AVS/AReMS Meeting, North Carolina State University, Raleigh, North Carolina — November 15, 2013.
6. **Poster presentation** for the SHPE National Conference, Indianapolis, Indiana — November 01, 2013.
    - Technical Poster and Paper Finalist at the Engineering Science Symposium
5. **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

4. **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
3. **Poster presentation** for the LSAMP Research Symposium at Cornell University, Ithaca, New York — August 07, 2012.

AEOLUS Unmanned Aerial Reconnaissance System by CU AIR

2. **Group presentation** for the Student Unmanned Aerial Systems Competition (SUAS) at Association for Unmanned Vehicle Systems International (AUVSI), Patuxent River Naval Air Station, Maryland — June 24, 2010.
    - Team awarded $1,000 grant

Academic Integrity

1. **Group presentation** for the Freshman Forum at Meinig Family Cornell National Scholars, Ithaca, New York — April 21, 2010.

Teaching Experience

Instructor — Springs 2023–2025 — EN.500.113: *Gateway Computing: Python*, Johns Hopkins University

This course introduces fundamental programming concepts and techniques, and is intended for all who plan to develop computational artifacts or intelligently deploy computational tools in their studies and careers. Topics covered include the design and implementation of algorithms using variables, control structures, arrays, functions, files, testing, debugging, and structured program design. Elements of object-oriented programming. algorithmic efficiency and data visualization are also introduced. Students deploy programming to develop working solutions that address problems in engineering, science and other areas of contemporary interest that vary from section to section. Course homework involves significant programming. Attendance and participation in class sessions are expected.

Instructor	Falls 2023–2024	EN.510.666: *Introduction to Computational Materials Modeling*, Johns Hopkins University

Moore's law has given rise to the silicon age, where computational modeling can provide high-fidelity predictions to address challenges spanning climate change and renewable energy to economic stability and global pandemics. The skills to solve scientific problems computationally have become invaluable in virtually all industries. This introductory course is project-based and puts into practice the fundamentals of software development, numerical analysis, and scientific programming. Topics covered include methods for solving differential equations, Monte Carlo and atomistic simulations, machine learning, and data visualization. The course is taught in Python, and support for non-UNIX architectures is limited.

Co-Instructor	Spring 2021	ME 555: *Applications of Artificial Intelligence in Materials*, Duke University Department of Mechanical Engineering and Materials Science

In this special topics course, AI principles will be applied to a series of materials science example problems, each taught in a module by an expert in materials science or data science. Each module spans 2-3 weeks, demonstrating an array of data science/AI methods in unique materials case studies in advancing discovery or design principles. Each module will have a homework assignment which will include application of AI methods to the module topic. No final exam. Pre-requisites: prior materials science course and prior AI/ML course; instructor permission.

Teaching Assistant	Spring 2020	ME 555: *Computational Materials Science by Examples and Applications*, Duke University Department of Mechanical Engineering and Materials Science

Graduate-level materials science course covering solid state topics such as conductivity and bands, quantum mechanics, and computational approaches for calculating materials properties.

Teaching Assistant	Fall 2014–Spring 2015	ME 221: *Structure and Properties of Solids*, Duke University Department of Mechanical Engineering and Materials Science

Introduction to materials science and engineering, emphasizing the relationships between the structure of a solid and its properties. Atomic and molecular origins of electrical, mechanical, and chemical behavior are treated in some detail for metals, alloys, polymers, ceramics, glasses, and composite materials.

- 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

The Louis Stokes Alliance for Minority Participation (LSAMP)	January 03, 2021	*Innovators and Trailblazers Magazine 2020* lsmrce.org/documents/community/LSAMP-Trailblazers-Magazine-2020.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
Diversity in Action	September 2018	*Options in Education: Building Bridges — Pratt School of Engineering mentors underrepresented students* bluetoad.com/publication/?i=521423&ver=html5&p=70
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
Duke University MEM Program	November 2013	*Society of Hispanic Professional Engineers* memp.pratt.duke.edu/news/society-hispanic-professional-engineers
New York Kiwanis	February 2013	*New York Kiwanis Mid-Winter Conference 2013* kiwanis-ny.org/1213/midyear.htm
ERN Conference 2013	February 2013	*2013 Oral and Poster Presentation Award Winners* new.emerging-researchers.org/2013-oral-and-poster-presentation-winners
New York Kiwanis	June 2012	*K-Kids Show Talent for Fundraising* patch.com/new-york/eastmeadow/k-kids-show-talent-for-fundraising

New York Kiwanis	March 2012	*Past Circle K Governors Help Celebrate 50th Convention* Elected Governor of New York Circle K. kiwanis-ny.org/news/view_news.php?nid=618

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
Award	November 09, 2018	Presentation Finalist at the Engineering Science Symposium, SHPE National Conference
Publication Award	2018	Editor's Choice, Publication in Comput. Mater. Sci., Elsevier
Award	November 03, 2017	Presentation Winner at the Engineering Science Symposium, SHPE National Conference
Publication Award	2017	Editor's Choice, Publication in Comput. Mater. Sci., Elsevier
Award	November 04, 2016	Presentation Finalist at the Engineering Science Symposium, SHPE National Conference
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
Fellowship	2013–2015	Associate Fellow, National GEM Consortium
Award	November 01, 2013	Technical Poster and Paper Finalist at the Engineering Science Symposium, SHPE National Conference
Award	August 22, 2013	Best Presentation Award at the MEMS Departmental Retreat, Duke University Department of Mechanical Engineering and Materials Science
City Citation	March 21, 2013	New York City Citation as Circle K Governor, Council Member Fernando Cabrera

Award	March 02, 2013	First Place in Nanoscience and Physics Research Presentation, NSF / AAAS / EHR Emerging Researchers National Conference
Award	October 08, 2011	College Bowl Winner, Hispanic Engineer National Achievement Awards Conference (HENAAC)
Scholarship	2011–2013	Shell Incentive Fund Scholarship
Honor	2010–2013	Louis Stokes Alliance for Minority Participation (LSAMP) Scholar
Scholarship	2010 & 2011	Xerox Corporation Scholarship
Scholarship	2010 & 2011	Intel Academic Award
Scholarship	2010–2013	GE Foundation / LULAC Scholarship
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)
Scholarship	2009	*Men of Principle* Award, Beta Theta Pi • Beta Delta Chapter
Scholarship	2009	Gold Medallion Winner in Engineering and Mathematics, Hispanic Heritage Youth Awards
Scholarship	2009	New Jersey Principals and Supervisors Association Scholarship
Scholarship	2009	Edward J. Bloustein Distinguished Scholar
Scholarship	2009	Investors Savings Bank Scholarship
Scholarship	2009	Bloomfield Education Association Scholarship
Scholarship	2009	Special Recognition Award, Bloomfield Kiwanis
Scholarship	2009	The Harold Brotherhood Award
Scholarship	2009	Jean Doswell Oakes Scholarship, Oakeside Cultural Center
Scholarship	2009	Superintendent's Bengal Pride Award for Excellence in Academics and Citizenship
Award	2009	Outstanding Student Citizen for Youth Week, Bloomfield High School
Award	2009	First Place Impromptu Essay, New Jersey Key Club Convention
Scholarship	2009	Good Citizen Award, The Daughters of the American Revolution
Honor	2008–2009	National Honor Society
Honor	2008–2009	Scholar Athlete, Bloomfield High School
Honor	2006–2009	Academic Excellence, Bloomfield High School
Honor	2008	National Ventures Scholar Program
Award	2008	Yale Book Club Award, Yale Club of Montclair, New Jersey

Certifications

Completion	June 5–6, 2023	National Science Foundation (NSF) Broadening Participation: 2023 Mathematical and Physical Sciences (MPS Workshop) for Young Investigators at the National Science Foundation
Completion	May 8–12, 2023	American Society for Engineering Education (ASEE) 2023 NSF Engineering CAREER Proposal Workshop Mock Panel Review Session at the American Society for Engineering Education

Completion	January 11–12, 2023	Center for Teaching Excellence and Innovation (CTEI) Best Practices in University Teaching Workshop at Johns Hopkins University
Training	September 20–29, 2022	Center for Teaching Excellence and Innovation (CTEI) Justice, Equity, Diversity and Inclusion (JEDI) Training Series at Johns Hopkins University
Graduate	June 25–29, 2018	Machine Learning Summer School (MLSS) at Duke University
Completion	September 26–29, 2017	*NextProf* Workshop at the University of Michigan
Graduate	January 7–16, 2015	Machine Learning Summer School (MLSS) at the University of Texas at Austin
Graduate	May 22–27, 2011	*The LeaderShape Institute* at Cornell University
Technician License	July 29, 2010	American Radio Relay League (ARRL) in Roselle, New Jersey

Activities and Outreach

Member	2022–present	The Minerals, Metals & Materials Society
Member	2014–present	American Physical Society
Faculty Advisor	2009–2018; 2023–present (hiatus 2018-2022)	Society of Hispanic Professional Engineers, Johns Hopkins University, Duke University & Cornell University
	Positions: Faculty Advisor, Graduate Student Advisor, President, Corporate Vice President & Treasurer	
Participant	2018–2024	Open Databases Integration for Materials Design (OPTiMaDe) Workshop, CECAM (Centre Européen de Calcul Atomique et Moléculaire)
Graduate Representative	2015–2018	Council of Presidents, Duke University Graduate School
Undergraduate Researcher	2011–2013	Brock Research Group, Cornell University
New York District Distinguished Past Governor	2010–2013	Circle K, Cornell University
	Positions: New York District Distinguished Past Governor, New York District Distinguished Past Treasurer & Restarting Chapter President at Cornell University	
Member	2009–2013	Meinig Family Cornell National Scholars, Cornell Commitment
Mechanical Engineer	2009–2011	Cornell University Autonomous Flight Team, Cornell University
	Constructed an autonomous plane with capabilities to navigate waypoints, survey areas, and retrieve visual information about the surfaces below as part of a team effort for AUVSI's (Association for Unmanned Vehicle Systems International) Student Unmanned Aerial Systems Competition. **Positions**: Mechanical Engineer, Safety Officer & Systems Manager	
President	2005–2009	Future Business Leaders of America, Bloomfield High School
	Positions: President & General Manager of School Store	
Membership Director	2005–2009	Key Club, Bloomfield High School
	Positions: Membership Director & Activities Director	
Retreat Team	2005–2009	Youth Group, Saint Thomas the Apostle Church
	Positions: Retreat Team, Lead Role in *Stations of the Cross Performance* & Confirmation Class Instructor	
President	2008–2009	Astronomy Club, Bloomfield High School
Member	2009	United Astronomy Clubs of New Jersey

Member	2009	New Jersey Astronomical Group, Montclair State University
Secretary	2006–2009	Model United Nations, Bloomfield High School
	Positions: Secretary & Treasurer	
Treasurer	2006–2009	Math Team, Bloomfield High School
Member	2006–2009	Science Club, Bloomfield High School
	Physics Club · Chemistry Club	
Athlete	2006–2009	Spring Track and Field, Bloomfield High School
	Javelin Junior Varsity Team	
Member	2006–2009	Weight Lifting Team, Bloomfield High School
Tutor	2006–2009	Tutor at the Library, Bloomfield High School
County Freeholder	2008	American Legion Jersey Boys State
	Positions: County Freeholder & City Councilman	
Member	2005–2008	Latin Club, Bloomfield High School
Member	2005–2006	Bowling Team, Bloomfield High School
Black belt	2002–2006	Tae Kwon Do, USMA in Clifton, New Jersey