
TCSUH Bi-Weekly Seminar

From Prediction to Design: Harnessing AI for Superhard and Multifunctional Materials Discovery

Prof. Jakoah Brgoch

Department of Chemistry and Texas Center for Superconductivity

Thursday, March 20, 2025

In Person – Room 102, Houston Science Center, 12:00 p.m. – 1:00 p.m

Sandwiches will be provided on a first-come, first-served basis.

ABSTRACT: Superhard materials, defined by a Vickers hardness greater than 40 GPa, are essential for applications ranging from manufacturing tools to energy technologies, where extreme mechanical performance is required. However, the discovery of new superhard materials has been limited by the difficulty of quantitatively predicting hardness from a material's composition and structure. To address this challenge, we developed an ensemble machine-learning model capable of directly predicting load-dependent hardness with high accuracy. We integrated this model with a machine-learning-driven phase diagram tool to efficiently search chemical spaces and identify promising candidate materials with superhard properties. Recognizing that many industrial applications involve extreme thermal environments, we further extended our approach to incorporate predictions of hardness at elevated temperatures and oxidation onset temperatures, enabling the search for materials that maintain performance under harsh conditions. As experimental validation, we synthesized and characterized a yttrium borosilicide compound predicted by our model to exhibit high hardness and excellent thermal stability. Mechanical property and thermal gravimetric measurements confirmed the model's predictions, demonstrating the power of machine-learning-guided discovery to accelerate the identification of novel superhard materials with the potential for real-world application.

BIO: Prof. Jakoah Brgoch is an Associate Professor in the Department of Chemistry and a Principal Investigator in the Texas Center of Superconductivity. Jakoah also has a courtesy appointment in the William A. Brookshire Department of Chemical and Biomolecular Engineering and is a member of the Hewlett-Packard Enterprise Data Science Institute. Jakoah completed his bachelor's and master's in chemistry from Illinois State University, followed by his Ph.D. from Iowa State University and Ames National Laboratory under the supervision of Gordon Miller, followed by postdoctoral research at the University of California, Santa Barbara in the Materials Research Laboratory with Ram Seshadri. Jakoah is now leading a multidisciplinary research group with research topics ranging from developing persistent luminescent materials for bio-imaging to understanding the mechanical response in superhard materials all through a combination of materials synthesis, characterization, first-principles computation, and machine learning. He has published over 100 peer-reviewed papers, earned a 2018 NSF CAREER research award, and was named a 2020 Alfred P. Sloan Research Fellow in Chemistry.
