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MACHINE LEARNING AND DATA SCIENCE IN MATERIALS RESEARCH (MLDSMR) SEMINAR SERIES

Dr. Wenhao Sun
Dow Early Career Assistant Professor
Materials Science and Engineering
University of Michigan Ann Arbor

Tuesday, October 8, 2024; 1 pm – 2 pm

Microsoft Teams

Join the meeting now

Meeting ID: 258 314 777 009

Passcode: G4GmoH

Computational Materials Discovery in the Age of AI and Robotics

Abstract: In the modern age of data science, there is more catalogued and query-able data than ever before. Here I will discuss how we can leverage high-throughput materials data from computational, experimental, and literature sources to accelerate the discovery of new functional materials. First, I will present a large stability map of the ternary metal nitrides, constructed using a suite of high-throughput computational materials discovery and informatics methods. Guided by our map, we experimentally realized a new class of ternary nitride semiconductors with tunable optoelectronic properties, expanding the palette of nitride semiconductors beyond Al/Ga/In-Nitrides. To more effectively design synthesis routes to computationally-predicted materials, we next demonstrate how Natural Language Processing algorithms can extract materials synthesis recipes from the scientific literature. By analyzing trends and anomalies in these published synthesis recipes, we hypothesized new design principles for highly-reactive precursors to complex multicomponent oxides. Using a robotic inorganic materials synthesis laboratory, we show that our predicted precursors substantially outperform traditional precursors. Robotic laboratories offer an exciting new platform for data-driven experimental synthesis science, from which we can develop new fundamental insights to guide both human and robotic chemists.

Bio: Dr. Wenhao Sun is the Dow Early Career Professor of Materials Science and Engineering at the University of Michigan. He double majored in Materials Science and Engineering and Applied Mathematics at Northwestern University, and obtained his PhD in Materials Science and Engineering from MIT. The Sun Research Group uses high-throughput density functional theory, applied thermodynamics, and materials informatics to deepen our fundamental understanding of synthesis–structure–property relationships, while exploring new chemical spaces for functional technological materials. Wenhao was named a 2020 Materials Horizons Emerging Investigator, and was awarded the 2020 Department of Energy Early Career Award, as well as the 2022 Camille and Henry Dreyfus Award for Machine-Learning in the Chemical Sciences.

For further information, please contact Dr. KT Tan at ktan@uakron.edu.