UCI Samueli School of Engineering

Department of Materials Science and Engineering UCI

UNIVERSITY OF CALIFORNIA, IRVINE

DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING

IS PROUD TO HOST A SEMINAR BY

"TOWARDS PREDICTIVE MATERIALS SYNTHESIS WITH ATOMISTIC SIMULATIONS AND ROBUST MACHINE LEARNING"

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UNIVERSITY OF CALIFORNIA, LOS ANGELES

Thursday, April 17, 2025

2:00 PM - 3:20 PM

McDonnell Douglas Engineering Auditorium

Abstract: In the last decade, numerous advances in materials design were made using databases, high-throughput screening, and machine learning (ML) approaches. While determining which structures should be synthesized is now a mature task, few theoretical approaches can predict how to synthesize them. In this talk, I will discuss how a unified view on entropy, simulations, and ML can enable predictive models for the synthesis of inorganic materials. First, I will discuss how high-throughput simulations can optimize both the synthesis and performance of new nanoporous catalysts. Building on these successes, I will describe how information theory can be used for a range of tasks in atomistic simulations relevant to synthesis prediction, from improving the robustness of ML models to modeling synthesis mechanisms and phase transformations. Finally, I will describe how generative ML can be used to generate complex amorphous structures, from glasses to mesoporous materials, thus integrating advances in artificial intelligence, materials theory, and simulations.

Bio: Daniel Schwalbe-Koda is an Assistant Professor of Materials Science and Engineering at UCLA. He was a Lawrence Fellow at the Physical and Life Sciences Directorate of the Lawrence Livermore National Laboratory, and received a PhD in Materials Science and Engineering from MIT in 2022. Some of his recent recognitions include the DOE Early Career Award (2024), a Scialog Fellow (2024), and the Forbes "30 Under 30" award in the Science category (2023).