

UNIVERSITY OF CALIFORNIA, IRVINE

THE DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING

Is Proud to Host a Seminar by:

**ASSOCIATE PROFESSOR
TAYLOR D. SPARKS**

Department of Materials Science
and Engineering
University of Utah



***MATERIALS INFORMATICS: MOVING BEYOND
SCREENING VIA GENERATIVE MACHINE
LEARNING MODELS***

DATE:

Thursday, December 7, 2023

TIME:

2:00 - 3:20 PM

LOCATION:

McDonnell Douglas Engineering Auditorium

Abstract: Machine learning already enables the discovery of new materials by providing rapid predictions of properties to complement slower calculations and experiments. However, a persistent criticism of machine learning enabled materials discovery is that new materials are very similar, both chemically and structurally, to previously known materials. This begs the question “Can machine learning ever learn new chemistries and families of materials that differ from those present in the training data?” In this talk, I will describe new generative machine learning approaches that can be used to generate structures that do not yet exist, but are likely to. I will compare generative models including variational autoencoders, generative adversarial networks, and diffusion models which have become standard in machine learning for images. I will describe the unique challenges that we face when using tools of this nature to generate periodic crystalline structures and I’ll also describe how tools such as DiSCoVeR and SMOCT can be used in conjunction to ensure chemically reasonable, yet interesting outputs.

Bio: Dr. Sparks is an Associate Professor of Materials Science and Engineering at the University of Utah and recently completed a sabbatical at the University of Liverpool with support from the Royal Society Wolfson Visiting Fellow program. He holds a BS in MSE from the UofU, MS in Materials from UCSB, and PhD in Applied Physics from Harvard University. He was a recipient of the NSF CAREER Award and a speaker for TEDxSaltLakeCity. He is active in MRS, TMS, and ACERS societies and serves as an Associate Editor for the journals Computational Materials Science and Data in Brief. When he’s not in the lab you can find him running his podcast “Materialism,” creating materials educational content for his YouTube channel, or canyoneering with his 4 kids in southern Utah.

