PHYSICS AND BIOENGINEERING COLLOQUIUM:
Machine Learning to Accelerate the Discovery of Energy Materials

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Date:
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Time:
10:30 AM-11:50 AM

Link:

Please contact snsgradstaff@ucmerced.edu for the Zoom link and passcode.

About The Speaker:

Linda Hung is a Senior Research Scientist in the Accelerated Materials Design and Discovery group at the Toyota Research Institute, where her research integrates machine learning with materials simulation and high-throughput experiment datasets. She has a background in computational materials science, with a focus on density functional theory, spectroscopy, and high-performance computing. She obtained her PhD in Applied and Computational Mathematics from Princeton University, and has held research positions at the Ecole Polytechnique (France), the University of Illinois Chicago, and the National Institute of Standards and Technology.

Abstract:

Machine learning (ML) provides a powerful set of tools for the study and discovery of new materials. At the same time, limitations of ML – including the need for a sufficiently large dataset to train a model, as well as difficulties in interpreting a model's range of validity – may prevent scientists from adopting it into their research workflow. In this talk, I will discuss how we integrate ML and materials science for our research and software tool development in the Accelerated Materials Design and Discovery group at TRI. After an overview of main research areas, I will highlight a few projects that demonstrate how machine learning can help our understanding of the physics of materials. These examples, which apply ML to X-ray absorption spectroscopy and density functional theory datasets, illustrate how incorporating scientific knowledge and theories can make ML more accurate and more interpretable.