UNIVERSITY OF CALIFORNIA, IRVINE

THE DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING

Is Proud to Host a Seminar by:

ASST. PROFESSOR ELIZABETH M.Y. LEE

Dept. of Materials Science and Engineering

University of California, Irvine

Thursday, October 13, 2022

2:00-3:20 PM

Location: McDonnell Douglas Engineering Auditorium

An Ab Initio Look At The Formation of Quantum Defects in Silicon Carbide and Molecular Dissociation Of Nitrogen On Ruthenium

Abstract: Engineering next-generation electronic devices, ranging from battery electrodes, photoelectrocatalysts, to solid-state quantum sensors, requires precise knowledge of how the structural arrangement of atoms impact the electronic properties of materials during synthesis and device operation. A promising tool for studying this is first-principles molecular dynamics (FPMD) based on density functional theory. However, these simulations are computationally expensive, which hinders their application. In this talk, I will discuss a computational modeling framework that combines FPMD with enhanced sampling and machine learning, to reveal electron spins and molecular reactions, as materials undergo electronic and structural changes. The first part will focus on the development of a neural network approach in simulating reactions in condensed phase systems. These algorithms enable the simulation of reactive processes, for instance, in the molecular nitrogen dissociation on metal catalysts, which is the rate-determining step in ammonia synthesis. In the second part, I will discuss modeling the high-temperature formation of quantum defects in solids to realize scalable quantum systems. This study reveals that understanding electronic structure and dynamics of spin defects are keys to designing new quantum technologies.

Bio: Elizabeth Lee is an Assistant Professor of Materials Science and Engineering and Samueli Faculty Development Chair at UCI. Her research centers on materials for energy and quantum technology applications to target both fundamental understanding and novel materials design using computational and theoretical approaches. Before coming to UCI, she was a postdoctoral scholar in the Pritzker School of Molecular Engineering at the University of Chicago, where she developed first-principles computational frameworks with neural networks to investigate chemical bonding dynamics and equilibria in quantum materials and metal surfaces. In her Ph.D. at the Massachusetts Institute of Technology, she studied nanoscale energy transport phenomena in molecular semiconductors, such as colloidal quantum dots and conjugated polymers, to design next-generation photovoltaics and LEDs. Her awards include DOE Leadership Computing Challenge Award, NSF Graduate Research Fellowship, American Institute of Chemical Engineers Electronics and Photonics Materials Award, and University of Chicago Maria Lastra Excellence in Mentoring Award.