IOWA STATE UNIVERSITY
Department of Mechanical Engineering

ME 600 Seminar

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November 30th at 11:00 am in 2004 Black

Title:

Computational Design of Functional Materials and Interfaces for Energy Storage and Conversion

Abstract:

A drastic switch to renewable energy storage and conversion technologies is required to meet the decarbonization goals of the Paris agreement as reinforced at COP26. There remain challenges with regards to the energy density, conversion efficiency, cost, integration, and scaleup of these technologies. Materials are at the forefront of these challenges and provide a promising route to achieve beyond incremental progress on these metrics. This talk will discuss how a combination of theory, computation, and data-driven methods can accelerate the design of functional materials and interfaces for two applications: solid-state lithium metal batteries and solar photovoltaics. The adoption of high energy density batteries based on lithium metal anodes has been hindered by the unstable and dendritic electrodeposition with liquid electrolytes, leading to safety concerns due to short-circuit. Solid-state batteries are safer, more durable, with better electrochemical, thermal, and mechanical stability than liquid electrolyte-based batteries. We discuss the prospect of enabling lithium metal anodes with solid-state batteries through fundamental results on the stability of solid-solid interfaces during electrodeposition. By incorporating the modification of the electrochemical kinetics due to mechanical stresses developed in the solid electrolyte, we identify a new paradigm of stability based on soft solid electrolytes that can lead to uniform electrodeposition. This regime is experimentally confirmed using a composite solid electrolyte designed such that its mechanical properties lie in the stability region. We further couple our design criteria with a machine learning framework developed for inorganic crystals to screen thousands of candidates, resulting in the discovery of new solid electrolytes. This talk will also discuss how first-principles simulations of surfaces, interfaces, and defects can provide valuable insights, not directly obtained using experiments, for hybrid organic-inorganic perovskite solar cells. We uncover the strong influence of surfaces and interfaces on material properties such as spin-orbit coupling and charge localization, which explains the discrepancies observed in the experimental literature. Finally, we propose ideal semiconductor interfaces for better charge transport and lower defect densities, leading to enhanced power conversion efficiency.

This seminar counts towards the ME 600 seminar requirement for Mechanical Engineering graduate students.

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