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Colloquium

Mechanical Engineering Lecture in Energy Science and Engineering

Computational materials design and interface engineering for renewable energy applications

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Nobel laureate Herbert Cromer once said of semiconductor technologies "The interface is the device." This sentiment is equally valid for many renewable energy technologies, including photovoltaics, thermoelectrics, fuel cells, electrolyzers, and batteries, in which device performance is governed by charge, ion, and/or thermal transport at interfaces. However, our limited understanding of interface structure-property-performance relationships remains a critical challenge in modern materials design.

In this talk, I will discuss our efforts to address this challenge by developing new approaches combining first-principles and molecular dynamics computations, neural network interpolation, and thermodynamic and kinetic modeling to understand, predict, and engineer interface phenomena. I will illustrate this approach primarily in the context of oxide-water interfaces for electrocatalytic H2 production. I will also highlight two examples in which we exploit interface phenomena to design new materials systems. In the first example, we make use of environment-dependent interface chemistry to design a dynamically tunable catalyst that enables low-temperature chemical CO2 sequestration; in the second, we design an interface-stabilized ferroelectric photovoltaic that exhibits both high-efficiency and high-power. Our work provides new insights into interface structure-property-performance relationships, which may dramatically accelerate development of new technologies.