MITMECHE

Colloquium

Mechanical Engineering Lecture in Energy Science and Engineering

Atomic-scale engineering of interface phenomena for renewable energy applications

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The ability to systematically design materials system from the atomic scale up could dramatically accelerate the development of new technologies for renewable energy generation, storage, and conversion. Many of the key challenges in designing materials in these areas arise from our limited understanding of how interfaces affect performance. For example, the efficiency of solar cells, batteries, fuel cells, electrolyzers, and thermoelectrics can be limited by interfacial phenomena such as charge transfer, ion diffusion, phonon or photon scattering, and chemical reactions.

In this talk, I will discuss our efforts to address these challenges by developing new approaches combining first-principles density functional theory computations and machine learning techniques to understand, predict, and engineer interface phenomena. I will show several examples of how we have used this approach to develop a fundamental understanding of the role of solid-liquid interfaces in governing photo- and electro-catalytic water splitting in a variety of systems, including metal alloys and transition metal oxides. I will also briefly highlight our recent work using interface properties to engineer novel photovoltaics with low recombination and high open-circuit voltage.