

Spring 2016 Lecture Series
Chemical & Biomolecular Engineering

**Materials design and the investigation of
interfacial chemistry and electronic
structure for solar fuel synthesis devices**



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The discovery of new materials and their organization into efficient nanoscale architectures can have transformative effects on modern energy conversion devices. This is especially true for solar-driven electrocatalytic devices for fuel production, which at present lack the required efficiency and product selectivity for commercialization. When a new promising material is applied, open questions inevitably present themselves regarding the atomic or nanoscale nature of the associated new interfaces. I will argue that generating a fundamental understanding of the electronic structure and chemical nature of interfaces in these devices is essential to push this technology forward. Interfacial processes lie at the origins of efficiency because: (1) interfaces are the source of electrochemical potential gradients (which are responsible for charge separation), and (2) interfaces comprise the active sites for reactions (which are required to drive selective chemical transformations).

In this talk, I will discuss my recent investigations of new materials and interfacial chemistry and electronic structure relevant for the design of solar fuel devices. First I will describe the discovery and characterization of new metal oxides and nanoscale architectures that enable the water oxidation reaction, a key and often limiting half reaction for solar fuel production. Next I will present work that emphasizes the use of simplified model systems to assess the physical origins of efficiency. Here, surface-sensitive spectroscopic and scanning probe techniques are used to study the electronic structures of active interfaces, and to characterize the surface chemistry of reactant molecules and molecular co-catalysts relevant for selective CO₂ reduction.

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