

Insights from Surface Science Studies into the Surface and Interface Properties of Photoelectrocatalysts for Solar Fuels

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A surface science approach can greatly advance understanding of the structure and reactivity of photoelectrocatalysts for solar fuels. This involves experiments using well-defined model catalysts under controlled conditions utilizing a range of spectroscopic techniques for characterization of surface and interface properties and the nature and reactivity of surface-bound species. I will discuss several of our recent studies, which include investigations of the effects of dopant incorporation on the structural and chemical properties of the α -Fe₂O₃(0001) surface for water oxidation catalysis, facet-dependent activity and stability of Co₃O₄ nanocrystals towards OER, and the interaction of water with GaP(110), a semiconductor that is known to enable selective CO₂ reduction to methanol in aqueous solutions of CO₂ and nitrogen-containing heteroaromatics. For water oxidation on α -Fe₂O₃, we found that Ni doping in thin films of model catalysts caused a new termination for the films and induced formation of more stable surface-bound OH groups. For the Co₃O₄ system, we used the well-defined morphologies of nanocubes and nanooctahedra to demonstrate that the (111) surfaces vastly out-perform the (100) surfaces for OER activity (overpotential and current density). Finally we have spectroscopically identified *in situ* the surface-bound species on GaP(110) associated with exposure to water using ambient pressure photoelectron spectroscopy (APPEs). These observations on model systems afford further analysis and discussion of the role of surface-bound species in mechanisms for catalyzed water oxidation and CO₂ reduction.

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