Mesoscale Priority Research Direction

Electrocatalysts: Active Sites and Interfaces of Clusters

Opportunity

There is a significant gap between our understanding of electrocatalysts at the atomic level to the micron scale. Catalyst sizes, geometry, defects, interfaces and charges all play key roles in determining reaction rates and selectivity, yet experiments are primarily led by heuristics or intuition.

Approach

Build and characterize well-defined multiscale catalyst structures and interfaces. Develop a fundamental understanding of the key roles of catalysts sizes, geometry, charge, and interfaces via simulation and experiment including the application of in-situ methods.

Meso Challenge

The challenge is to prepare and identify active sites (or active interfaces across a wide range of dimensions and compositions) and understand how we can purposely build practical catalysts with the selectivity and rates we desire.

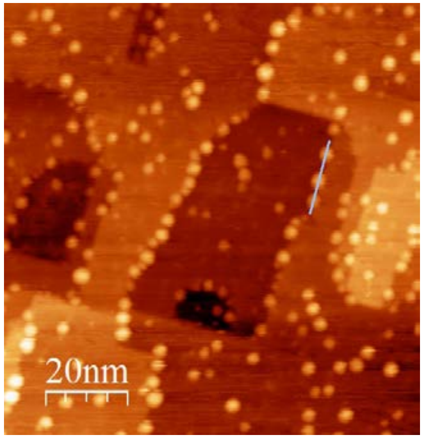
Impact

Novel catalysts and methods to upgrade basic chemical feedstocks (water, CO_2) to fuels using renewable energy (thermodynamically uphill reactions, electrochemical or photoelectrochemical) . Development of practical (low-cost) electrocatalysts for efficiently converting fuels to electrical energy (fuel cells).

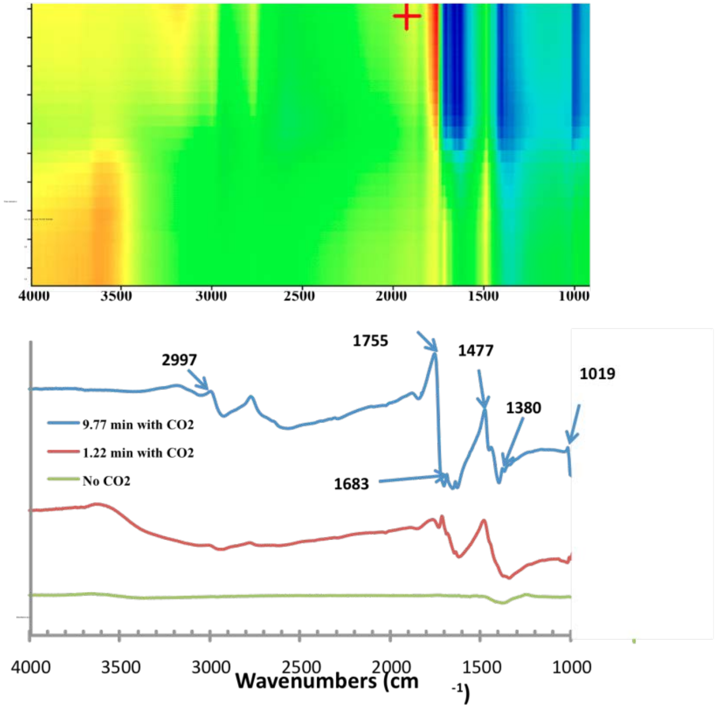
U.S. DEPARTMENT OF ENERGY | Office of Science

Contact: John Flake (johnflake@lsu.edu)

Electrocatalysts for CO_2 Conversion to Fuels



Cu nanoclusters on conductive metal oxide (ZnO) electrodes



In-situ FTIR showing intermediates in the reduction pathway.

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