U.S. DEPARTMENT OF
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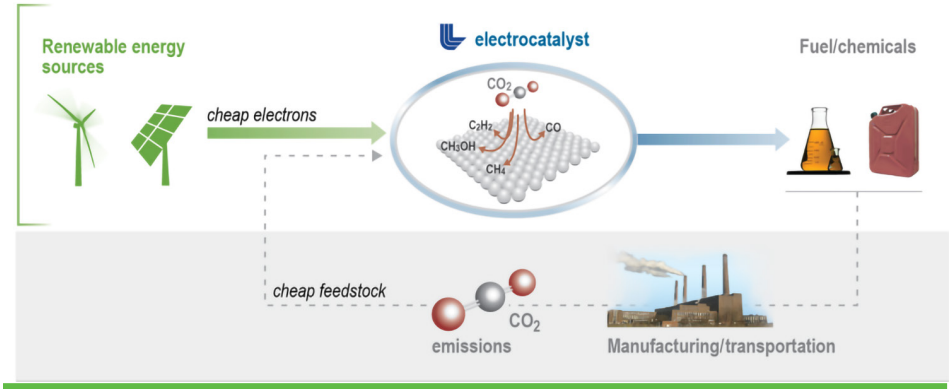
Rational Design Platform for Transition Metal Catalyzed Electrochemical Synthesis



Using electric energy from renewable energy sources, the copper-based electrocatalysts developed through this project would enable one-step conversion of CO_2 to methane and other versatile fuels and feedstock chemicals.

Graphic image courtesy of Lawrence Livermore National Laboratory

The increasing supply of low-cost electric energy from renewable sources such as wind and solar power is expanding the potential for new processes that convert electricity into chemical energy for grid energy storage, fuels, and chemicals. Grid energy storage is one of the immediate priorities for electrosynthetic chemical production, but needs to overcome some technical barriers to be widely deployed. While batteries can be used as a short-term storage medium, they are a relatively high cost and inefficient option for long-term energy storage, limiting their practicality for seasonal storage. "Power-to-Gas" (PtG) conversion of electricity to chemical energy is becoming an increasingly attractive long-term storage option. Chemical energy offers safe long-term storage and could be readily dispatched using existing infrastructure to meet required demands.

The most widely used PtG technologies convert electricity to hydrogen through water electrolysis, followed by carbon dioxide (CO_2) methanation. These reactions are energy-intensive and rely on expensive platinum-based catalysts. A promising alternative PtG process is the one-step electrochemical reduction of CO_2, currently produced primarily from the combustion of fossil fuels, to methane and other fuels, which has the potential to significantly reduce capital and process costs compared to current state-of-the-art PtG approaches. If efficient low-cost electrocatalysts can be effectively integrated, then the electrochemical PtG technology could potentially offer a viable option for converting abundant renewable electricity into valuable chemicals.

This project focuses on harnessing the unique electrocatalytic activity of inexpensive copper (Cu) based catalysts to convert CO_2 to methane and other versatile fuels and feedstocks. Among available candidates, copper shows promise as an earth-abundant replacement for more expensive noble metal catalysts operating at mild pressures and temperatures. To incorporate Cu-based catalysts into this process, researchers will integrate materials synthesis and quantum simulations to develop a full understanding of the catalytic mechanism and energetics of this CO_2 to fuel conversion. Manipulating the potential energy landscape through tuning the composition, morphology, and environment of the Cu-based catalyst will improve the energy efficiency and selectivity needed for this PtG process.

Benefits for Our Industry and Our Nation

Harnessing the advantageous properties of copper in this electrochemical PtG technology could facilitate energy-efficient production of methane or other hydrocarbons with high selectivity and long-term stability. Expected process improvements include:

- Increased catalyst surface area by more than 10 times, which will increase the number and density of active sites
- Increased catalyst reactivity and selectivity for hydrocarbon formation by 10%

Applications in Our Nation's Industry

The conversion of abundant renewable-based electrical energy to chemical energy for grid energy storage, fuels, and chemicals is potentially attractive to utilities and chemical manufacturers. Methane is a preferred storage medium because it is relatively safe to handle and can be readily stored and integrated into existing pipelines for use in buildings, industry, and vehicles and also can be used for power production. In addition, this innovation could facilitate new selective pathways to produce higher value hydrocarbons and chemicals that are not currently accessible. Furthermore, this technology could enable another productive use for existing CO_2 streams with high purity.

Project Description

The project objective is to improve the energy efficiency and selectivity of copper-based catalysts for electrochemical CO_2 to fuel conversion. Researchers will integrate advanced theory, synthesis, and characterization capabilities to obtain a greater fundamental understanding of the mechanism of CO_2 reduction reaction (CO_2RR) on nanostructured copper and dilute copper alloy electrocatalysts. They will apply this understanding toward rational design of a tailored catalyst platform for PtG applications that then can be leveraged toward designing catalysts for other hydrocarbon products.

Barriers

- Integration of brittle hierarchical nanoporous copper catalyst materials into existing electrolyzer designs
- Long-term stability of electrode's nanoporous structure under electrochemical reaction conditions

Pathways

This project targets efficient and selective production of methane and other valuable hydrocarbons from CO_2 using nanoporous copper-based electrocatalysts. To optimize catalyst performance, researchers will optimize catalyst design by tuning (1) catalyst morphology, (2) composition, and (3) environment.

Phase 1 will integrate model catalyst development, synthesis, and characterization focusing on tuning catalyst morphology and composition. Modeling efforts will characterize the potential energy landscape along the reaction path for both pure copper and dilute alloy catalyst surfaces. Goal is to predict the onset potential of CO_2 reduction reactions. During this phase, both pure and dilute alloy nanoporous copper catalysts will be synthesized and characterized to test model predictions. The most promising catalysts will be further tested.

The second phase will develop the capability to predictively tune the catalyst environment to further increase selectivity and energy efficiency. The most promising catalysts will also be tested under varied environmental parameters, including pH, buffer capacity, and additives. The findings will guide future catalyst design efforts in the one-step electrochemical conversion of CO_2 to fuels.

Milestones

This two-year project began in May 2018.

- Synthesize and test pure nanoporous copper catalyst electrodes for catalytic activity, and select 1-3 catalyst morphologies for further study (Completed)
- Synthesize and characterize at least two different compositions of nanoporous dilute copper alloys with high agreement between predicted and observed ordering in overpotential and selectivity for further evaluation (Completed)
- Deliver novel catalyst with significant increase in current density along with increased selectivity toward hydrocarbons compared to existing two-dimensional copper catalysts (2020)

Technology Transition

This work leverages expertise at the Lawrence Livermore National Laboratory (LLNL) in synthesizing and characterizing tailored nanoporous dilute alloy catalysts and large-scale quantum simulations of electrochemical interfaces. LLNL is partnering with Opus 12, Inc., which brings expertise in CO_2RR catalyst testing and scaling to commercial quantities, and TOTAL American Services Inc, which brings industry insight on electrochemical CO_2 reduction to target molecules. Successful completion of this work can accelerate testing of these novel catalysts in a commercially relevant environment.

Project Partners

Lawrence Livermore National Laboratory
Livermore, CA
Principal Investigator: Dr. Juergen Biener
Email: *biener2@llnl.gov*

Opus 12, Inc.
Berkeley, CA

TOTAL American Services Inc
Hopkinton, MA

For additional information, please contact

G. Jeremy Leong
Technology Manager
U.S. Department of Energy
Advanced Manufacturing Office
Phone: (202) 586-3910
Email: *Jeremy.Leong@ee.doe.gov* ■

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