Electrons to Molecules at NREL: Renewable Chemical Technologies

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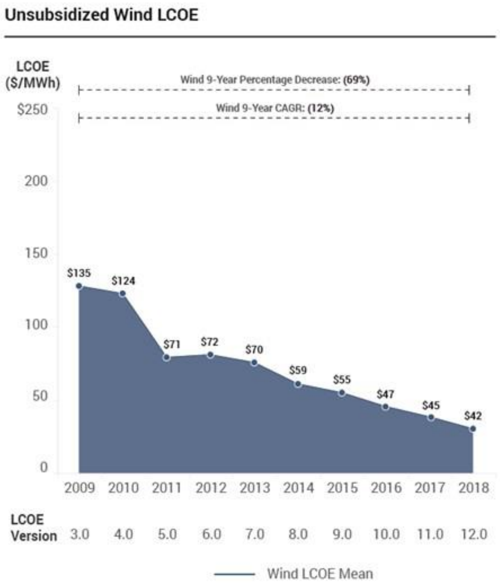
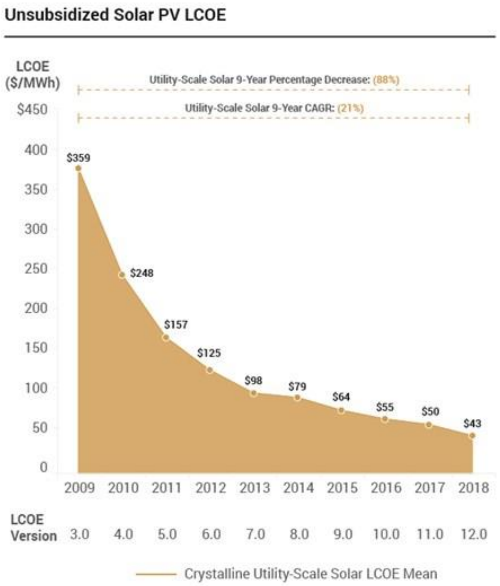
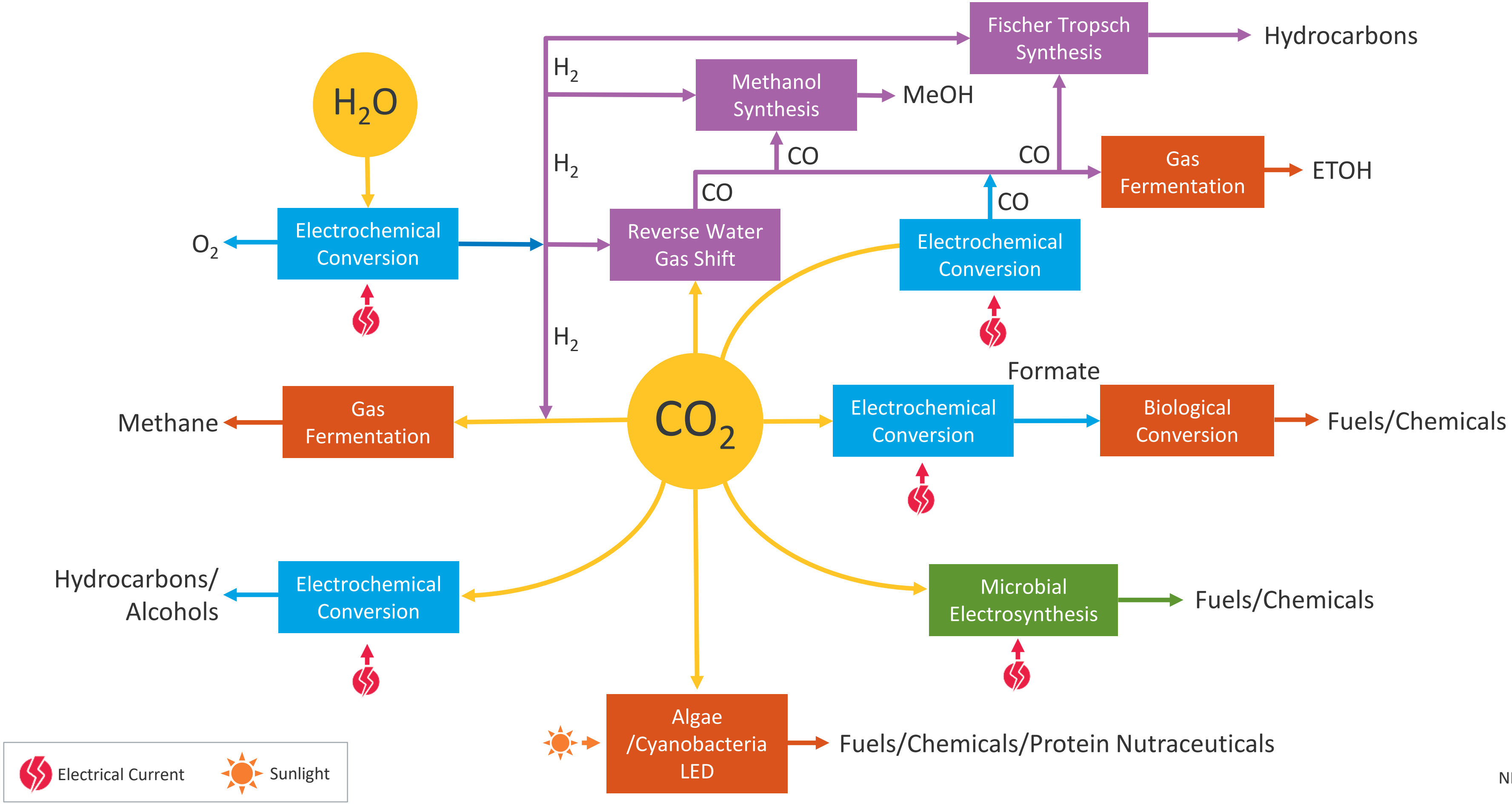
Strategic Lead for Electrons to Molecules
October 22, 2020

Downward Trends for Renewable Electricity Costs





E2M CO_2 Conversion Pathways



E2M - CO_2 Reduction and Utilization

$$H_2O \xrightarrow[\textit{Electrolysis}]{\Delta H^\circ\ \ 242\ \text{kJ/mol}} H_2 + 1/2O_2$$

- Leverages Program work from FCTO, BES, etc

$$CO_2 \xrightarrow[\textit{Electrocatalytic reduction}]{\Delta H^\circ\ \ 283\ \text{kJ/mol}} \underbrace{CO \xrightarrow{\Delta H^\circ\ \ 2\ \text{kJ/mol}} CH_2O_2 \xrightarrow{\Delta H^\circ\ \ -92\ \text{kJ/mol}} CH_3OH}_{\Delta H^\circ\ \downarrow\ C_2+} \xrightarrow{\Delta H^\circ\ \ -115\ \text{kJ/mol}} CH_4$$

- Targets building C-C bonds from intermediates of CO_2 reduction
- Targets novel hybrid approaches (with or without H_2)

Outcome: New ***concepts, approaches***, and understanding for chemical (carbon-carbon) bond formation using CO_2 and electrons through electro-catalysis, synthetic biology and advanced hybrid processes

Potential Impact

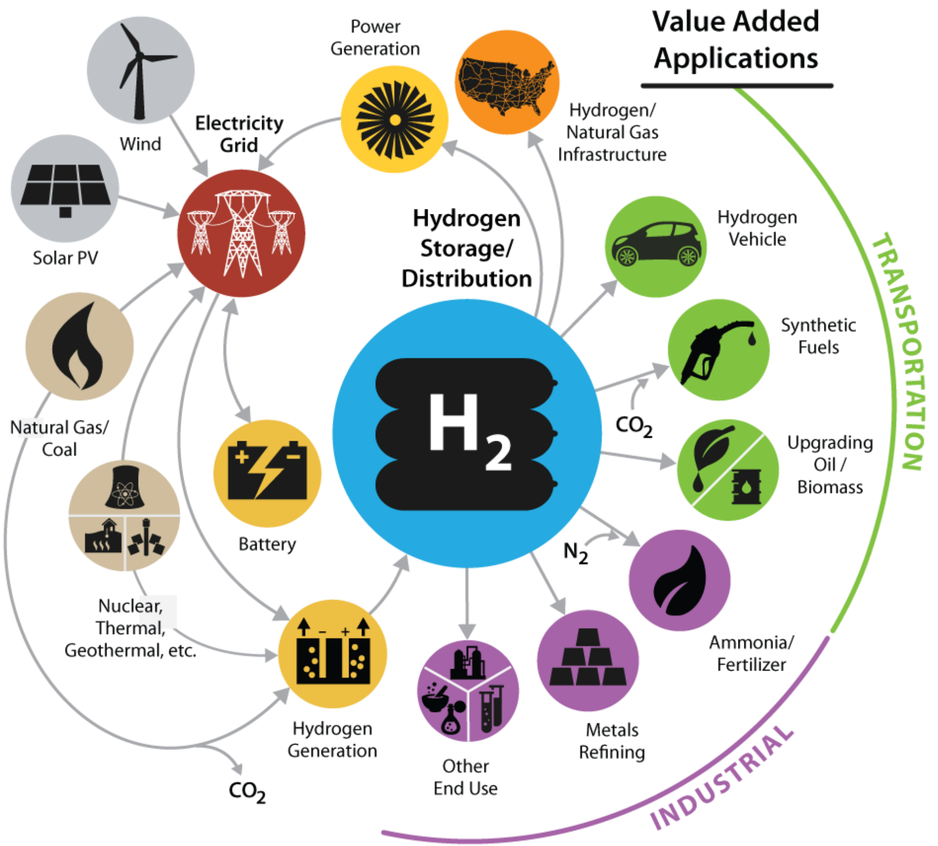
- Promotes CO_2 utilization and valorization
- Provides alternative route to products through low-cost electricity
- Chemical storage option

Conceptual H2@Scale Energy System

H2@Scale

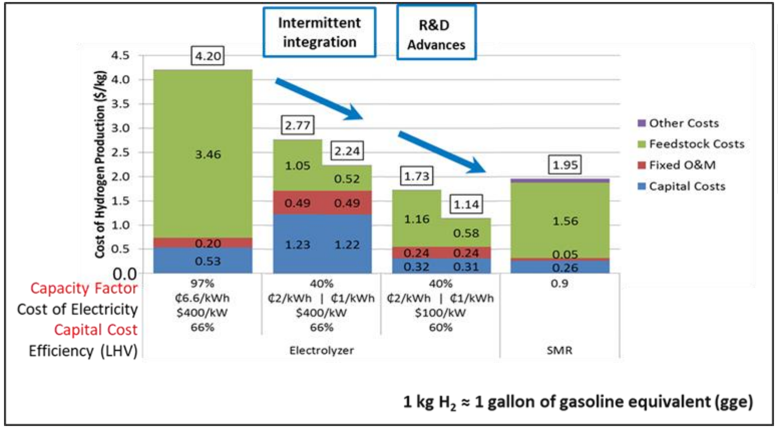
- Explores the potential for wide-scale H_2 production
- Enable resiliency of the power generation and transmission sectors
- Aligning with diverse Industries such as metal refining, ammonia, chemicals, and fuels upgrading

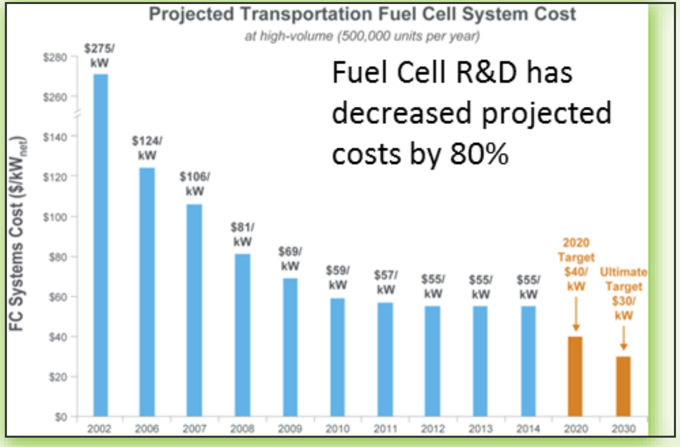
H2@Scale website:
http://energy.gov/eere/fuelcells/h2-scale



Illustrative example, not comprehensive

Pathway to Economical Generation of H_2 by Electrolysis





Hydrogen by Electrolytic Splitting of Water

- Near – Term Deployment for use in a variety of industries.
- Requires further cost reductions that may be overcome by scale.

Research and Development Needs

Electrocatalysts
- Improved performance and durability

Membranes
- Resistance to differential pressures/cycling
- Alkaline systems

Durability/Testing
- Degradation mechanisms; accelerated testing

Cell/Electrode Layer
- Impact of operating conditions
- Electrode structure/performance
- Manufacturing/Scale-up

Bipolar Plates/Porous transport layers
- Structure/performance; Corrosion
- Manufacturing/Scale-up

Balance of Plant
- Lower cost power supplies, inverters; DC systems
- High temperature compatible materials
- Impact of operating conditions

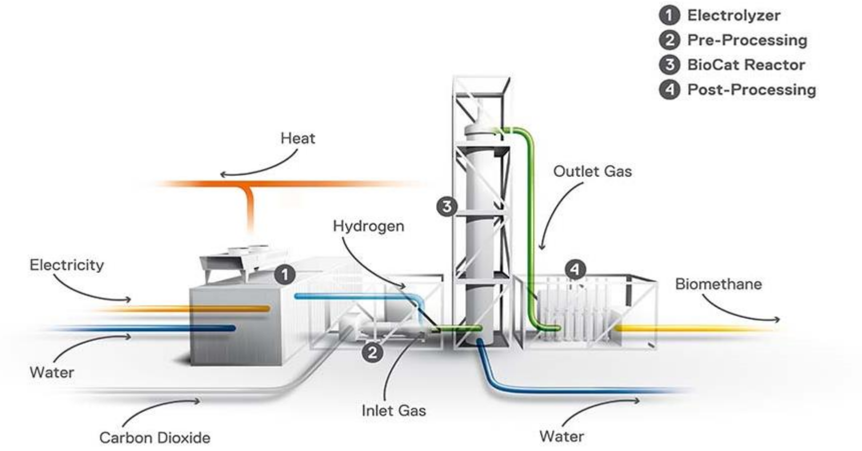
Renewable Methane Production

Scientific Approach

- Utilize excess electricity production for the electrolysis of water to H_2 and O_2
- Optimized strain of methanogenic archaea to perform methanation under industrial conditions
- 98% Carbon efficiency of CO_2 to CH_4
- Post-processing for pipeline quality natural gas

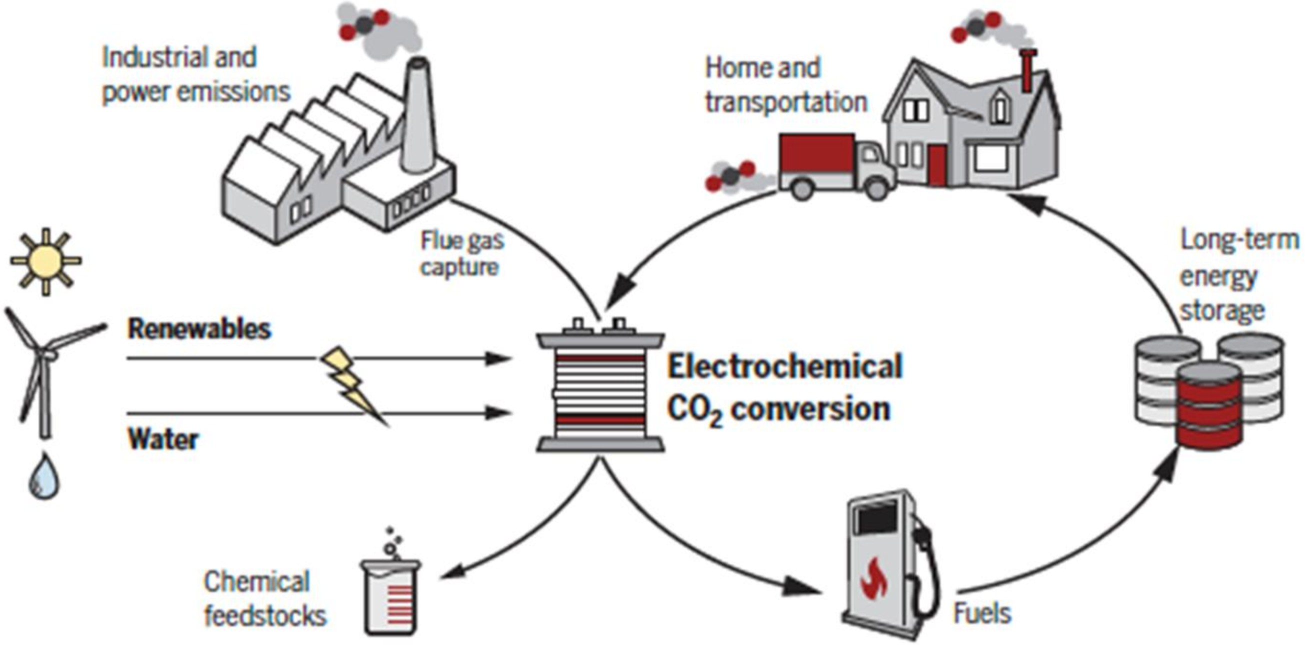
Significance and Impact

- Potential long term storage strategy via conversion of electricity & CO_2 to CH_4
- High efficiency CO_2 capture and conversion strategy
- Demonstrated route to renewable methane



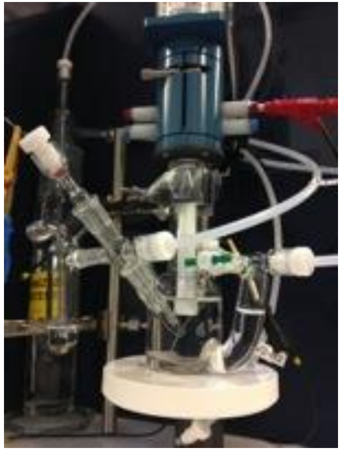
$$4H_2 + CO_2 \xrightarrow{\text{Biocatalyst}} CH_4 + 2H_2O + \text{Heat}$$

Electrochemical CO2 Reduction: Where are we now?



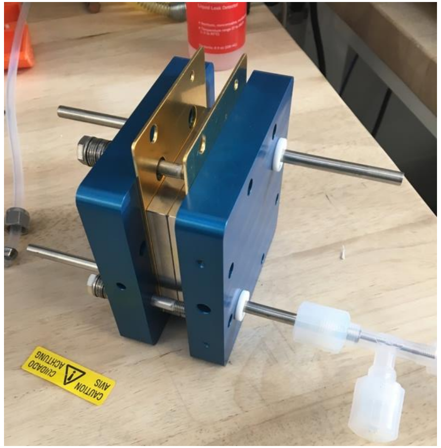
NREL’s Multi-Scale Electrochemical Capabilities

Rotating Disk Electrode



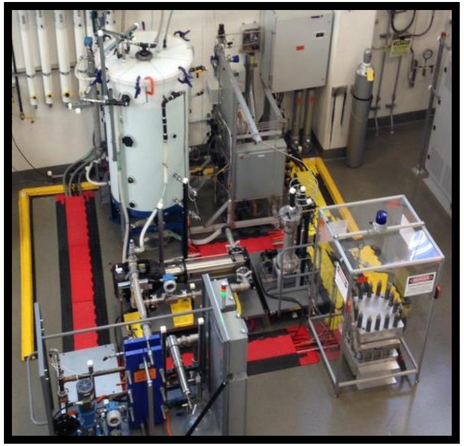
MilliWatts

Flow – Through Single Cell



Watts

Flow – Through Stacked System



KiloWatts

World Class Test Stations

GC with sampling manifold

HPLC with autosampler

Current Capabilities

- Anode and cathode can flow liquid (0-100 mL/min) or gas (0-4 SLPM)
- In-line automated gas sampling (two Agilent 490 MicroGCs)
  - H_2 , CO, CH_4, C_2H_4, CO_2
- HPLC with autosampler for liquid product analysis
- PEEK-PTFE backpressure (0-60 psig) regulators optimized for dual-phase flow
- Ambient to 85 °C operation
- Safety N_2 purge
- Flammable gas leak detection
- Enclosure ventilation exceeds NREL standard for chemical fume-hoods

Future Plans

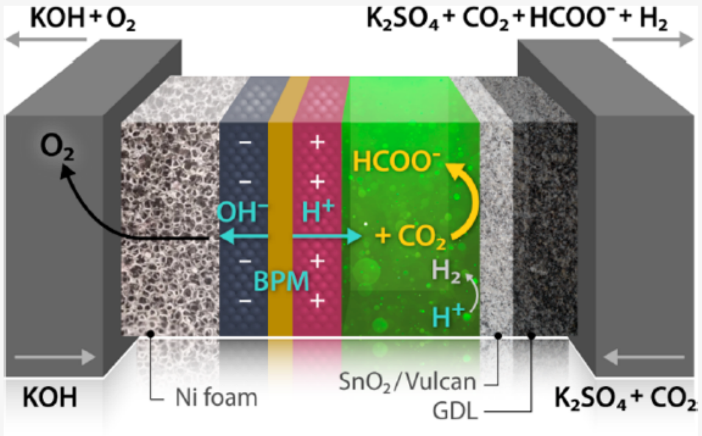
- Four additional stations designed for maximum modularity and ease of and maintenance/modifications
- Time-of-Flight – Mass-Spectrometer
  - Real time product analysis

Formate: Identifying Pathways to Higher Energy Efficiencies

Yingying Chen, Ashlee Vise, W. Ellis Klein, Firat C. Cetinbas, Deborah J. Myers, Wilson A. Smith, Todd G. Deutsch, and K. C. Neyerlin*

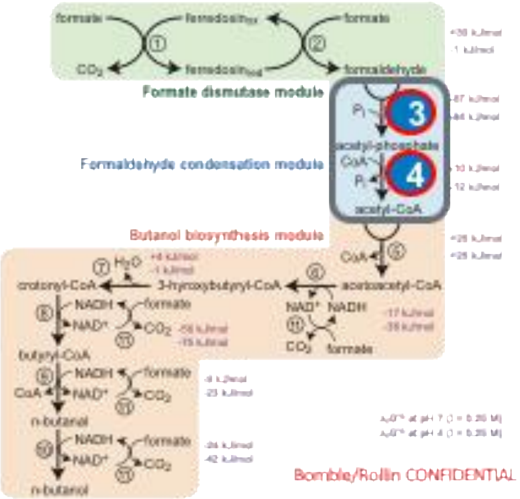
Cite This: *ACS Energy Lett.* 2020, 5, 1825−1833

ABSTRACT: This work demonstrated a robust, scalable cell architecture for electroreduction of CO_2 (CO_2R). An up to 90% faradaic efficiency for the conversion of CO_2R to formate at 500 mA/cm^2 was realized at a 25 cm^2 gas diffusion electrode (GDE) with a carbon-supported SnO_2 electrocatalyst. A 1.27 mm thick catholyte was used between the bipolar membrane and cathode GDE, which could be further reduced to tens of micrometers upon refinement. The deconvolution of the potential drop from each individual component/process guides the pathways to higher energy efficiencies of CO_2R at this platform. Significant changes in the agglomerate size and aspect ratio on the electrode before and after an 11 h test were revealed by nano-CT, suggesting reduced CO_2 accessibility from electrode degradation. The versatility of this CO_2R testing platform enables the ability to assess materials, components, and interactions at scales more in line with future devices.



Scientific Approach

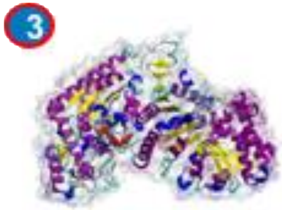
- Cell free approaches can be directly coupled to electrocatalytic production of formic acid from CO_2. The same electrolyser can be used to recycle CO_2 formed in enzymatic reactions.
- We can leverage enzyme promiscuity to convert formaldehyde to essential intermediates such as acetyl-phosphate and acetyl-CoA
- Focus on *Formaldehyde condensation* and *Butanol biosynthesis* modules and use rational design to engineer enzymes for increased stability, enhanced selectivity, and formaldehyde tolerance.



Significance and Impact

- An estimated 2.85 Gt CO_2 and 300 TWh ($0.02/kWh) are available for utilization each year.
- Developing approaches to convert these feedstocks to liquid fuels or biochemicals using excess electrons will promote efficient energy storage.

Phosphoketolase



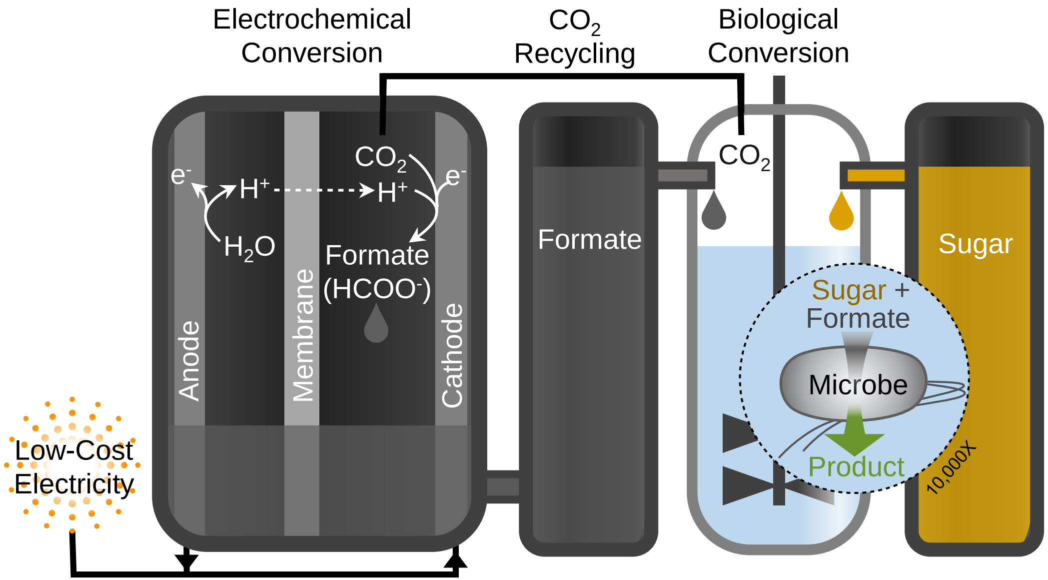
Phos-photransacetylase or Acetyltransferase

Partners

This project will benefit from a collaboration with Global Bioenergies S.A. and Philippe Marliere from Scientist of Fortune.

Electrochemical reduction of CO_2 to improve sugar conversion

- We envision a system in which CO_2 emitted during biological conversion is recycled by electrochemically reducing it to generate formate.



- Formate can be stored and used as an auxiliary energy source to improve biological conversion **for a wide variety of hosts, products and processes**.

Thank you

www.nrel.gov

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NREL is a national laboratory of the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, operated by the Alliance for Sustainable Energy, LLC.

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