Low-temperature Electrochemical Activation of Ethane for Co-production of Chemicals/Fuels and Hydrogen

WBS 2.1.10.2

Idaho National Laboratory/Massachusetts Institute of Tech/Univ of Wyoming

Project Period: May 2018-April 2020

Principal Investigator: Dong Ding, Ph.D
Idaho National Laboratory

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Overview

Timeline

- Project Started on May 2018
- Projected End date April 2020
- Project 7% complete

Barriers

Ethylene production via ethane steam cracking is energy-intensive and represents the most energy-consuming single process in chemical industry.

Budget

	FY 18 Costs	FY 19 Costs	FY 20 Costs	Total Planned Funding
DOE Funded	$200 K	$500 K	$ 300K	$ 1,000 K
Project Cost Share	$52 K	$125 K	$73 K	$250 K

Project Teams and Roles

- Dr. Dong Ding, INL
  - Oversee the entire project
  - Development of electrochemical cells/membrane reactor
  - Catalyst incorporation
  - Electrochemical testing
- Prof. Ju Li, MIT
  - Modeling and simulation
  - Advanced Characterizations
- Prof. Maohong Fan, Univ. of Wyoming
  - Catalyst R&D towards ethane deprotonation/ethylene coupling

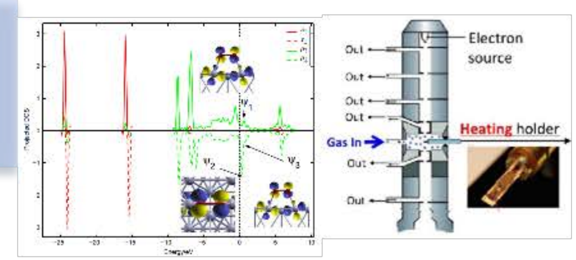
Objectives

- Overall Goal
  - to fully exploit the potential of natural gas and natural gas liquids with 50% energy reduction (AMO goal in 10 years) and lower carbon emissions. Specifically, our goal is to achieve a process energy efficiency of 90%, corresponding to a process energy reduction of over 65% compared to the industrial ethane steam cracking, and a product selectivity of 90%.

Demonstrate the proof of concept for co-production of chemicals/fuels and H_2 using ethane through a non-oxidative electrochemical deprotonation process at reduced temperatures

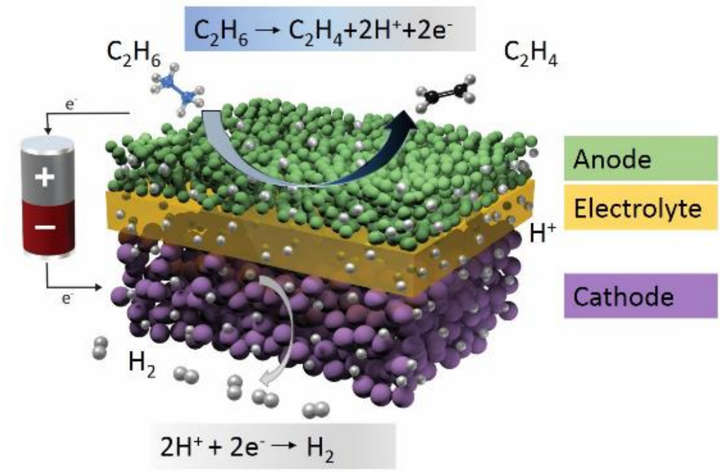
Develop new electrocatalysts that can be incorporated into electrochemical cells and have excellent catalytic properties towards ethane oxidation and ethylene coupling

Implement advanced modeling and characterizations for rational design of materials/components



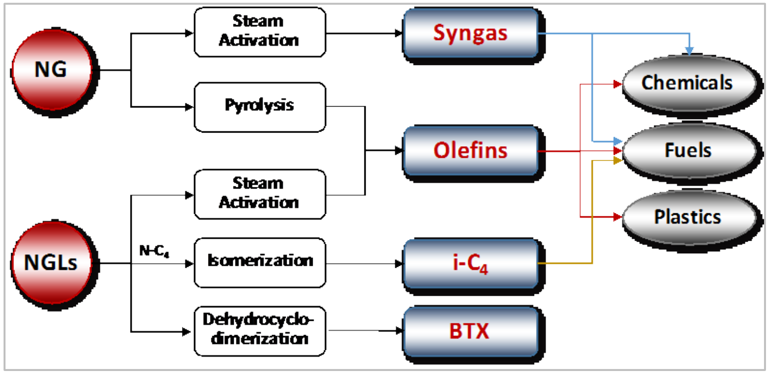
Technical Innovation

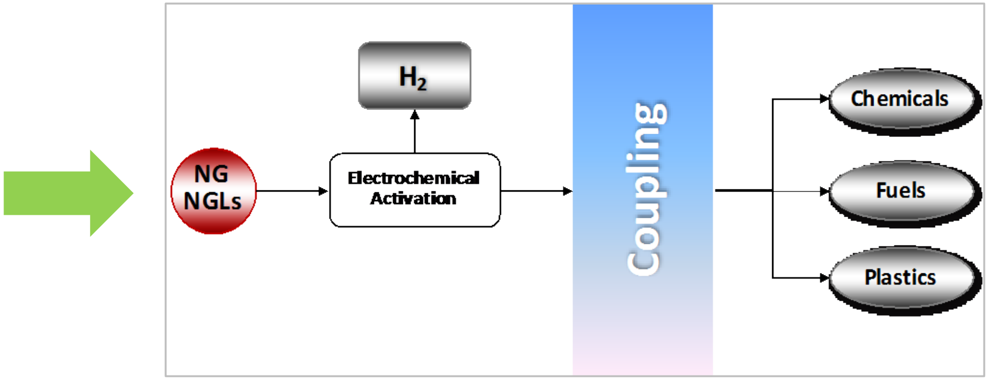
- ## State of the art:
  - Steam cracking, an energy-intensive method that contributes 60% of the final product cost and 65% of the manufacturing carbon footprint
  - Catalytic dehydrogenation, which has a thermodynamic limitation
  - Oxidative dehydrogenation, for which the product is easier to react than feedstock and increases CO_2 byproduct



- ## Proposed technology:
  - electrochemical process: overcome thermodynamic limitation, thus operating at lower temperatures;
  - Electrochemical membrane reactor: push the reaction forward by fast removal of H_2;
  - Intermediate temperature operation: Good balance by avoiding precious metal catalyst use at LT and alleviate fast degradation at HT;
  - Solid oxide cell: Modularity and can be readily incorporated with renewable energy

- ## Impact:
  - Providing a disruptive approach for petrochemical manufacturing, shifting the paradigm from thermal chemical practice to a clean energy regime;
  - High potential to secure U.S. industrial competiveness in chemicals, fuels and plastics manufacturing

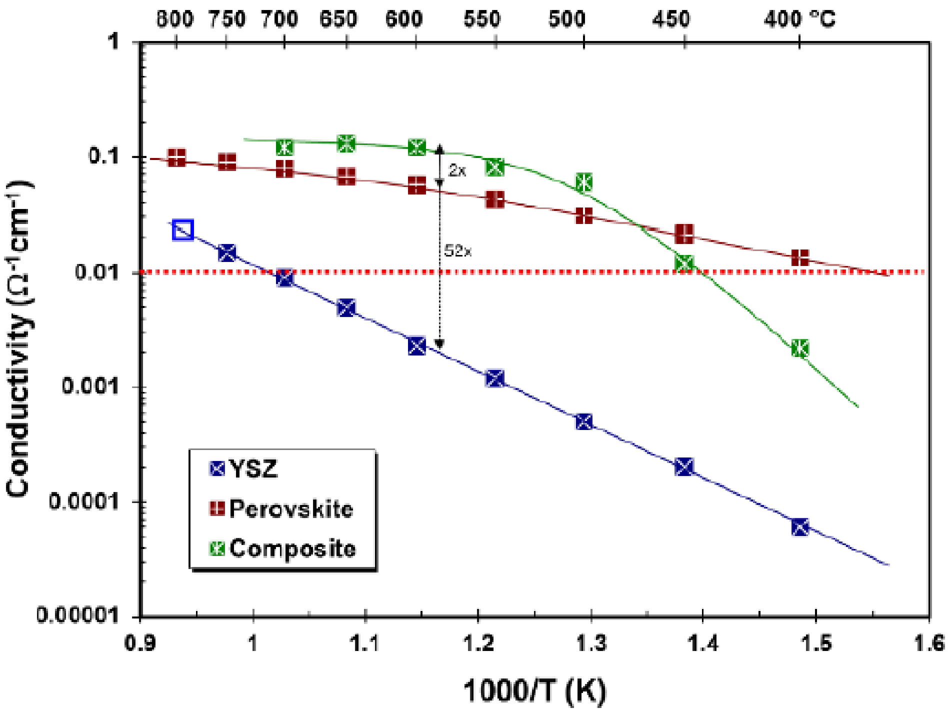


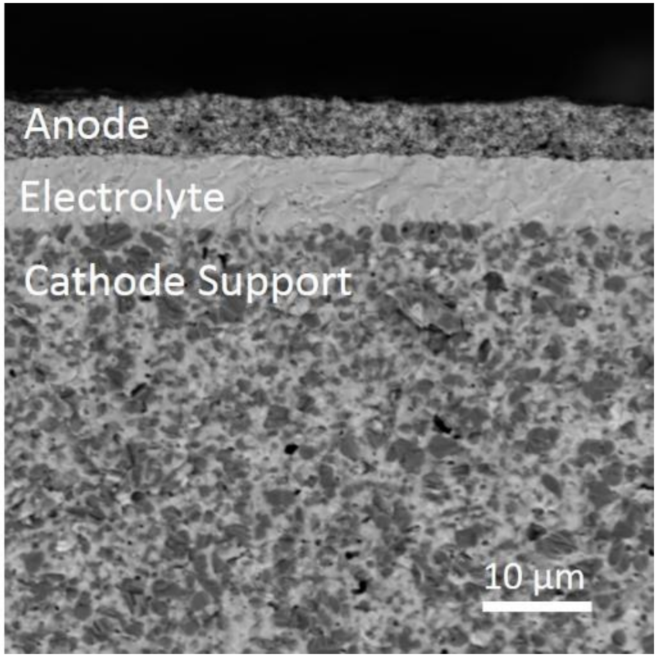


Technical Approach: Materials Perspective

Fast protonic conductors:
- High conductivity
- Low activation energy

Dense electrolyte membrane:
- Product separation
- Reduced Ohmic resistance





1. T He, US patent 2013;
2. D Ding et al, International Journal of Hydrogen Energy, 2014
3. D Ding et al, Journal of Power Sources, 2015

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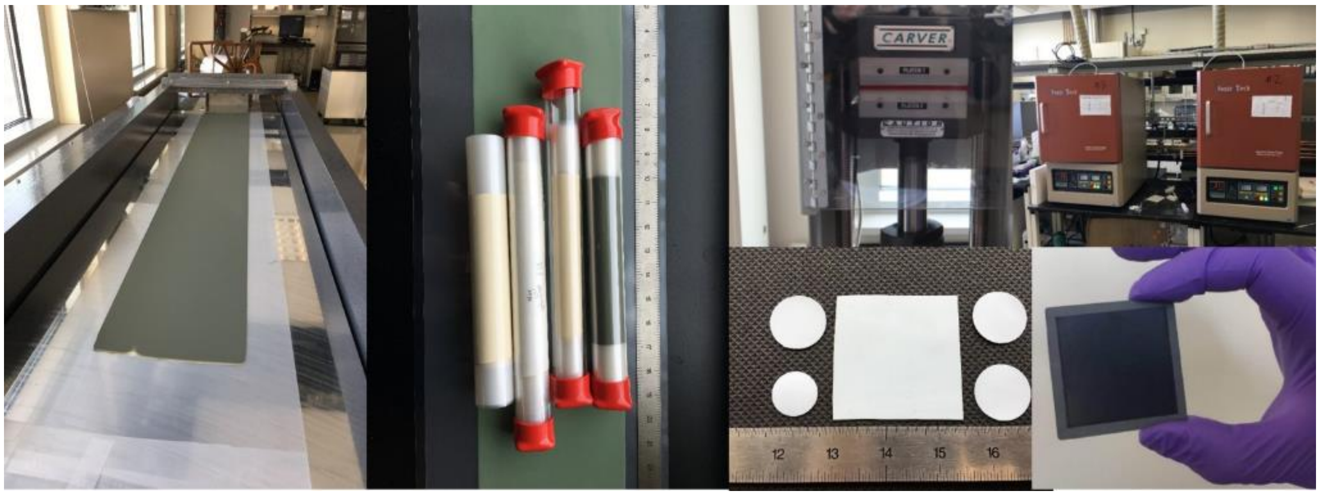
2. D Ding et al, International Journal of Hydrogen Energy, 2013
3. D Ding et al, Advanced Energy Materials, 2013

Technical Approach: Fabrication & Testing

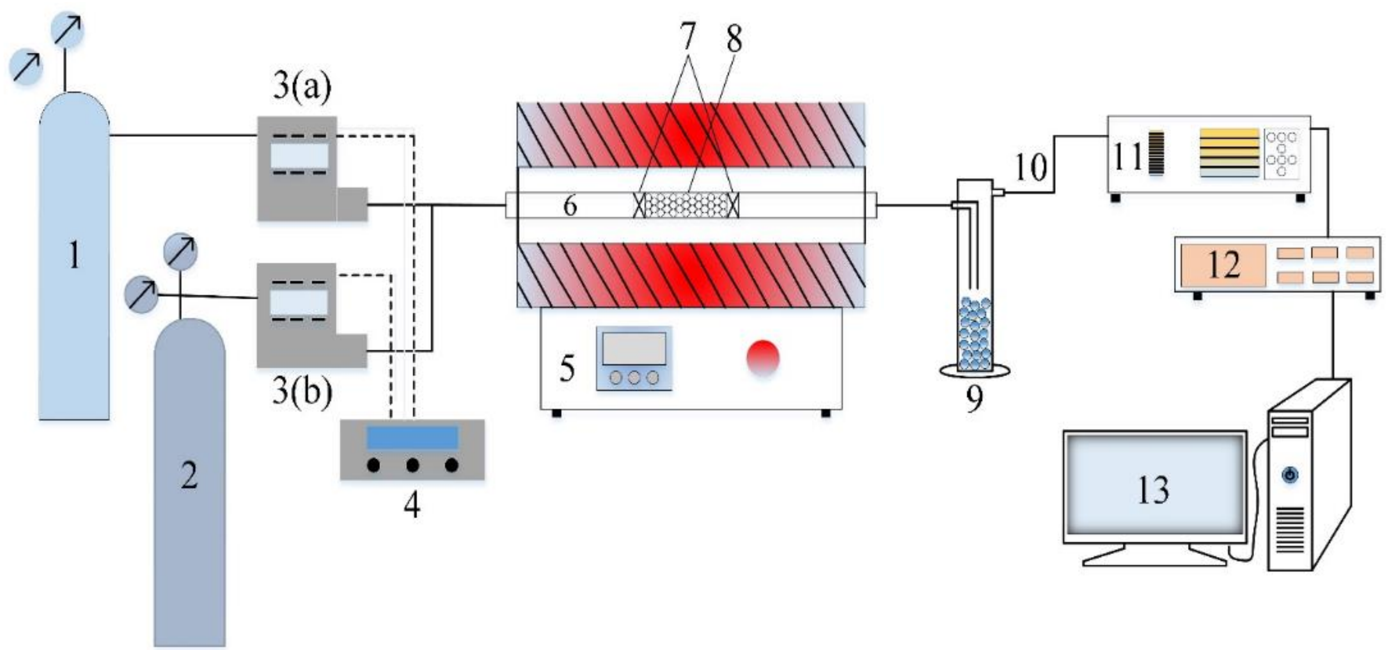
HT Roll-to-Roll Manufacturing for button cells to large planar cells



High Throughput materials testing/screening

Research Plan: Catalyst Development (UWy)

- **Task 1: Development of advanced ethane oxidation and hydrogen evolution catalysts**
  - Target is to achieve a process with high ethylene selectivity (> 90%) and ethane conversion.
  - Task 1 includes reactor design, preparation of the catalysts, catalyst structural characterization tests, and performance evaluation.
- **Task 2: Development of advanced catalysts for ethylene coupling**
  - Goal is to develop effective coupling catalysts for production of C_{4+} hydrocarbons (butylene, gasoline, or diesel) from ethylene.
  - Task 2 includes preparation of the catalysts, catalyst structural characterization tests, and performance evaluation.



Research Plan: *Ab initio* modeling & in situ TEM (MIT)

Modeling:

Protonic electrolytes: Energetics of polaron formation and migration in state-of-art electrolytes e.g. $BaCeO_3$, $BaZrO_3$ and BZCYYb; better mechanistic understanding of proton conduction and electrolyte stability.

Catalysts: Modeling electrocatalysis of ethane oxidation and hydrogen evolution; providing suggestions for better catalysts

In situ TEM:

Facility: FEI Titan environmental transmission electron microscope (ETEM) operated at 300 keV

Materials: Proton conductor supported nano-catalysts for ethane oxidation and ethylene coupling

Targets: Dynamic change of particle morphology and elemental distributions, especially at interface under operation conditions

Transition

This project will play a critical role in attracting industrial partners for product development and commercialization

- Successful execution of the project will significantly reduce commercialization risk by demonstrating the project goals are attainable.
- The project will increase the technology readiness from TRL2/3 to TRL-4.
- Some industry investors have shown their interests on this technology since it was highlighted by the AMO website. Collaborations and/or agreements are underway.

Questions?