Opportunities to enhance safe chemical manufacturing with electrochemical processes

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PURDUE UNIVERSITY | Davidson School of Chemical Engineering

About Me

Education & Background

BS Chemical Engineering,
University of Pittsburgh ***(2009 – 2013)***

PhD Chemical Engineering,
Columbia University ***(2014 – 2019)***
Advisor: Jingguang Chen
(Electrocatalysis & Sustainability)

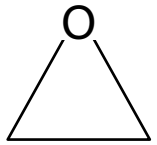
NRC Post-Doctoral Fellowship,
NIST ***(2019 – Aug. 2021)***
Advisor: Tom Moffat
(Electrochemistry Fundamentals)

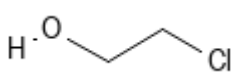
Asst. Prof. Chemical Engineering,
Purdue University ***(Aug. 2021 –)***

"NIST is a sort of acropolis of the average"

Hazards of Industrial Oxidation Processes

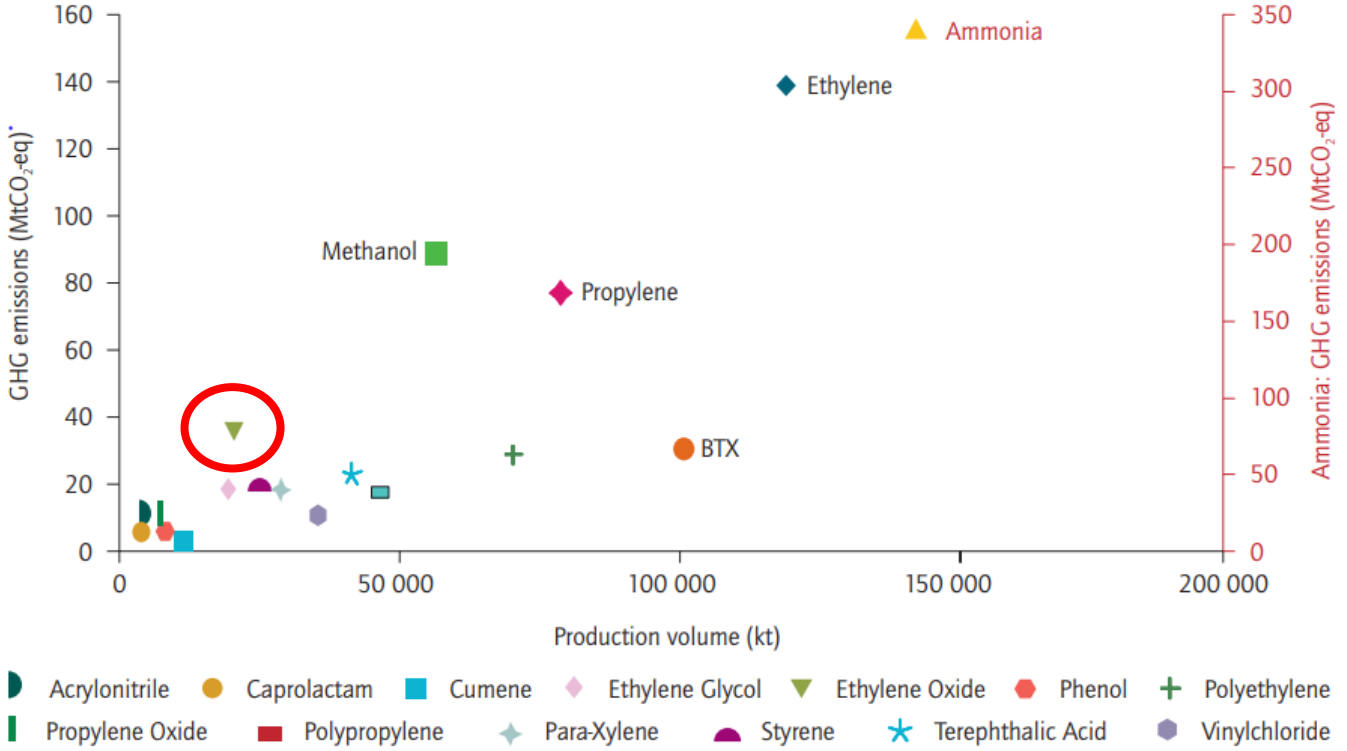
Case Study: Ethylene Oxide Synthesis



- Route 1: ***Direct Oxidation***
  - $C_2H_4 + O_2 \rightarrow C_2H_4O + CO_2$
    (from over-oxidation/gas compression)
  - ~10% single pass conversion @ 200 – 260 C, ~20 bar
    - Higher T, above flammability limit
- Route 2: ***Chlorohydrin Process***
  - $C_2H_4 + Cl_2 + H_2O \rightarrow$ 

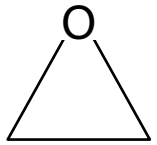
 $+ Ca(OH)_2 \rightarrow C_2H_4O + CaCl_2 + H_2O$

EO is a high-value, high-volume product with large CO_2 footprint



An Electrochemical Alternative

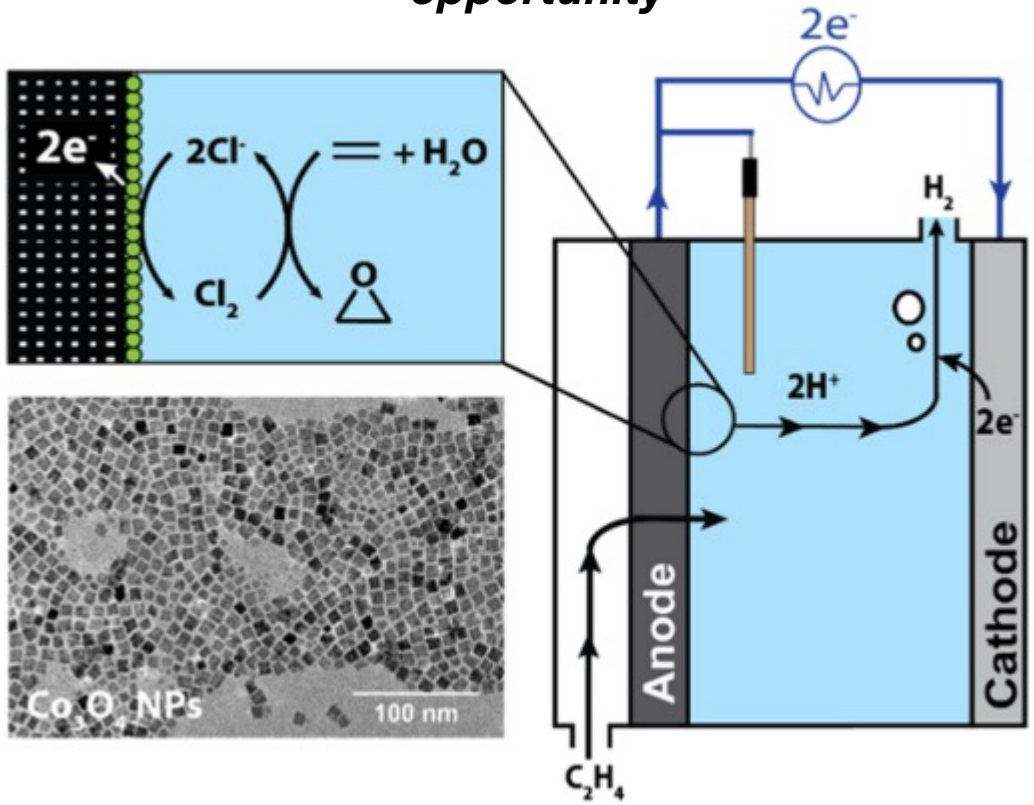
Case Study: Ethylene Oxide Synthesis



Can we synthesize EO more efficiently without handling toxic chemicals or risking explosions?

- Chlorine mediator is generated electrochemically at an electrode by electron transfer from aqueous Cl^- salt
- Cl_2 and H_2O transform ethylene to EO in the same manner as chlorohydrin process
- ***Resulting Cl^- ions are recycled as mediators (no stoichiometric waste)***
- Occurs @ 90 C

Electrochemical reactors provide unique opportunity



Chung, M., Jin, K., Zeng, J. S., & Manthiram, K. (2020). ***ACS Catalysis***, ***10***, 14015–14023.

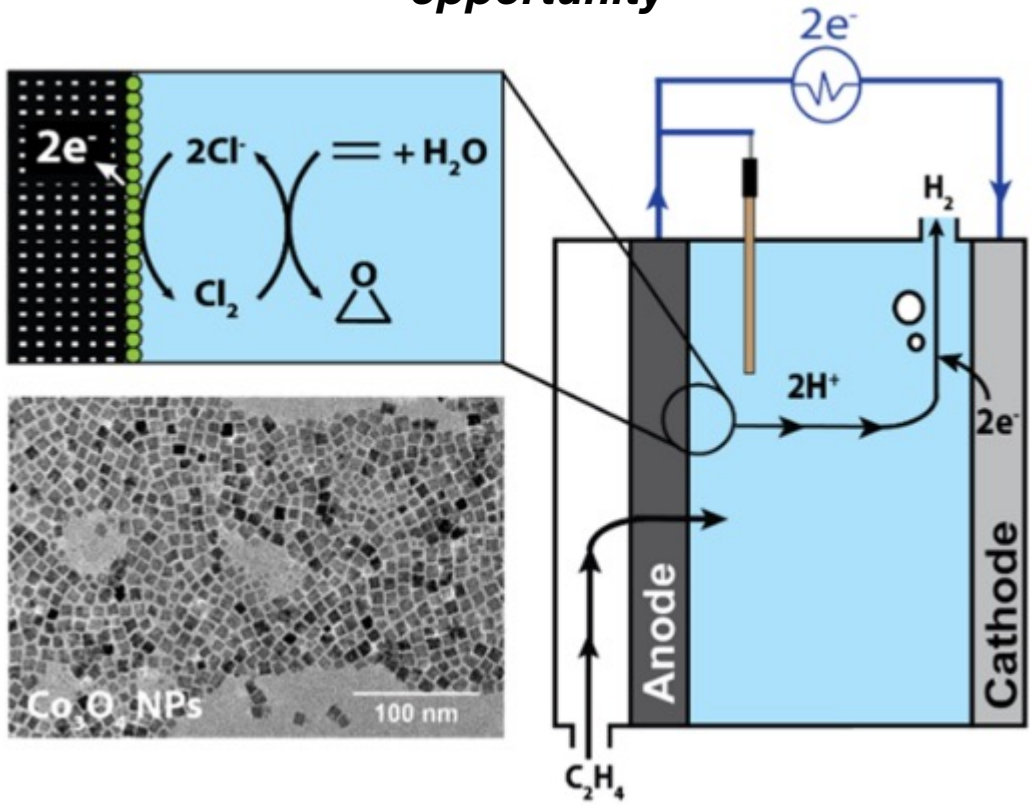
An Electrochemical Alternative

General Advantages of Electron-Driven Reactions

- Driving force for chemical reaction = electrochemical potential (i.e. voltage)
  - Facilitates ambient T processes
  - Enables finer selectivity control
- Reaction rate ∝ current
  - Quantifies rates accurately (10^{-12} mol/s)
- Electrodes are versatile
  - Conduct charge to redox mediators
  - Catalyze reaction directly (enhance activity/selectivity)

These enable selective oxidations that can potentially mitigate hazards in chemical processing

Electrochemical reactors provide unique opportunity



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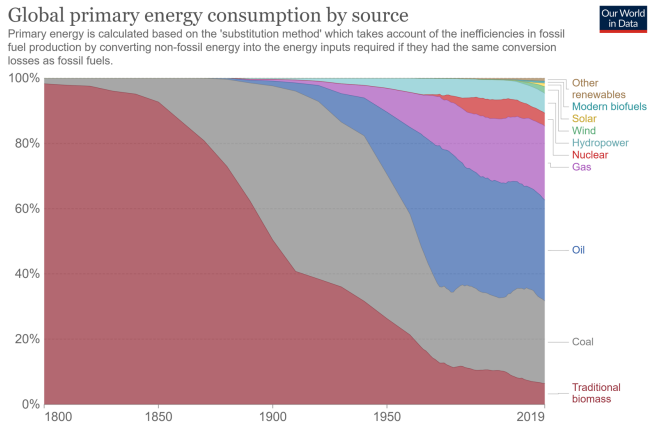
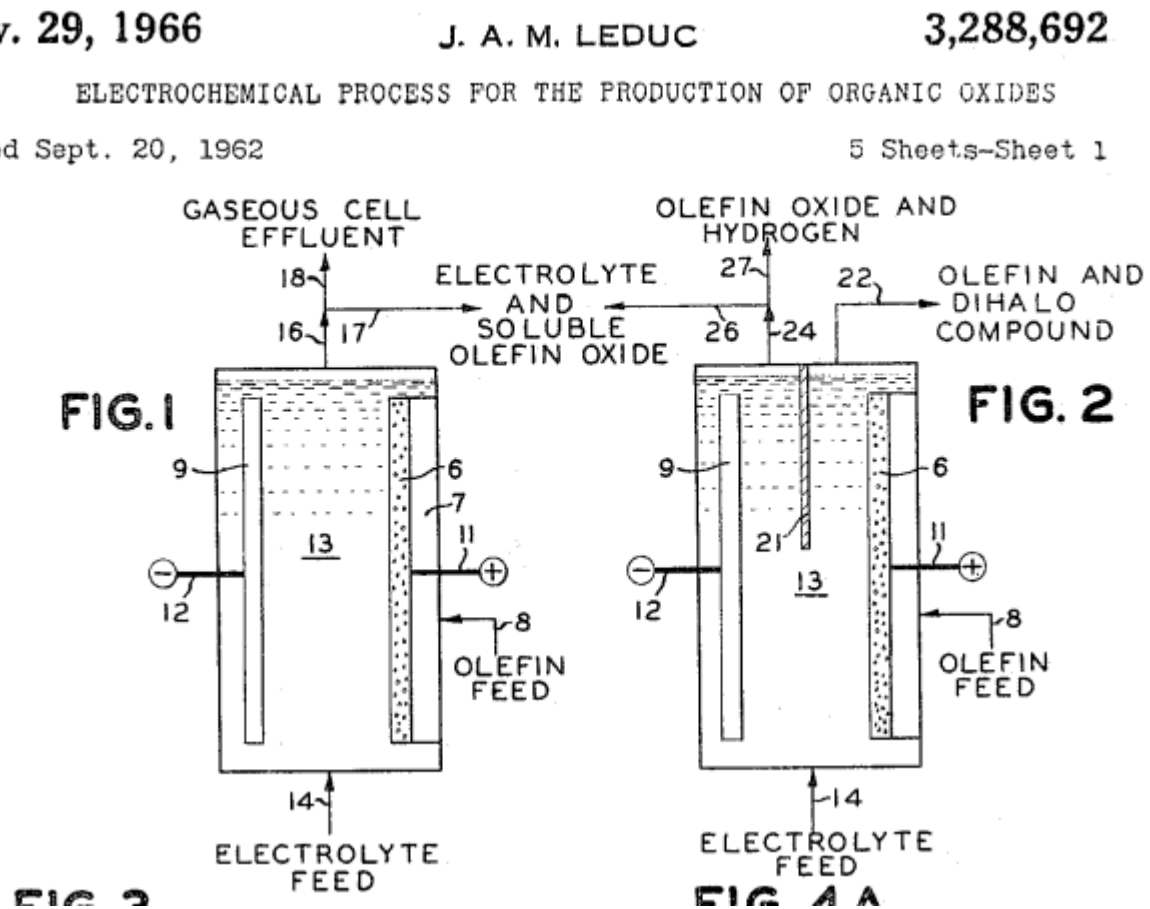
Why, What, and How?

Why Now?

- Electrochemical process have been around a long time
- Rapidly increasing abundance of electrons originating from wind/solar are motivating electrification, broadly
- Many great ideas from the past are now more economically/thermodynamically attractive

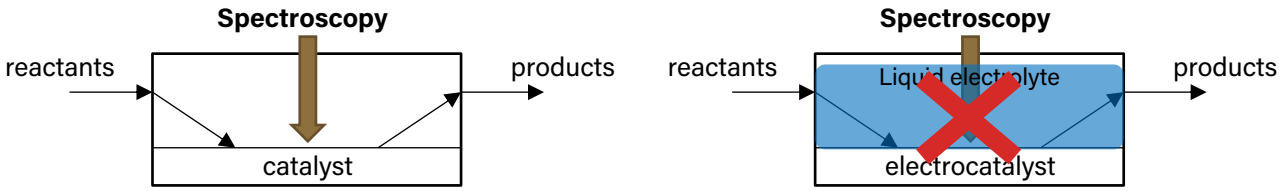


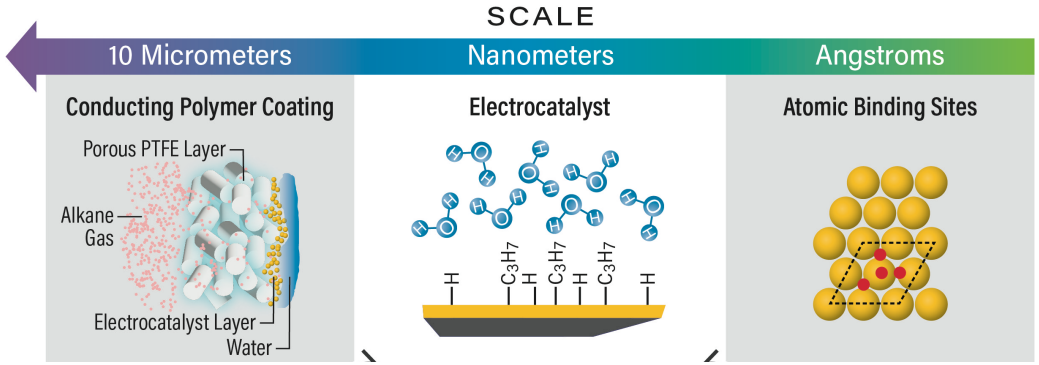


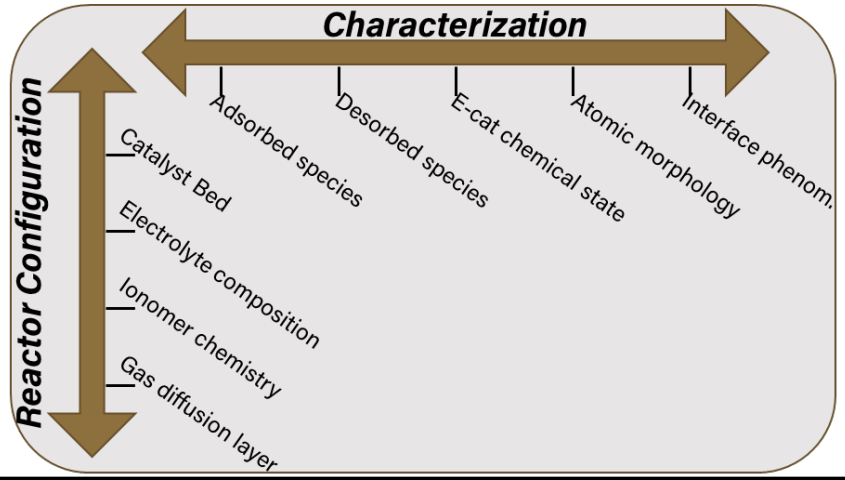
Why, What, and How?

What Do We Need to Realize This Vision?

- ***Characterization:***
  - Catalyst/reactor techniques developed over previous decades typically **not suitable for *gas-liquid-solid* interfaces commonly found in electrocatalysis**
  - ***Need:*** New/modified characterization techniques specifically designed for electrocatalysts (EC-MS, SEIRAS)
- ***Reactor Configuration:***
  - Electrocatalysts do not stand alone – **they are influenced by: *conductive current collector supports, gas diffusion layers, ion transport media (ionomer), electrolyte, membrane, etc.***
  - ***Need:*** Holistic approach to reactor design/analysis
- ***Education:***
  - Chem/ChemEs are best suited to pursue these problems, but **lack of training results in large depth/breadth of electrochem. manufacturing challenges to address**
  - ***Need:*** Integrated curriculum that presents electrochemistry along with Chem/ChemE core





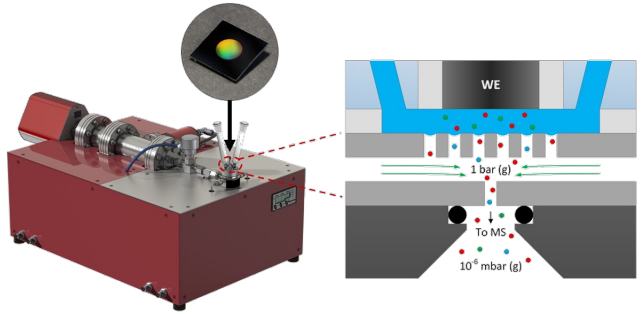


Why, What, and How?

How Am I Approaching These Challenges?

- My lab has a unique combination of characterization techniques that enable study of a wide array of electron-driven chemical reactions

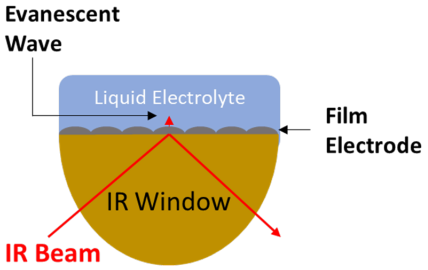
Electrochemical Mass Spectrometer (EC-MS)



- Fast (~1 s) and sensitive (100% product collection) gaseous product analysis
- Inert or reactive gas dosing capabilities

Ideal for fundamental studies of desorbed species

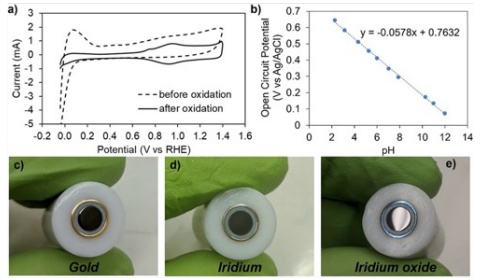
Surface Enhanced Infrared Absorption Spectroscopy (SEIRAS)



- Plasmon-enhanced vibrational spectroscopy captures near-surface signals
- Compatible with deposited film electrodes

Ideal for fundamental studies of adsorbed species

pH-Sensing Rotating Ring Disk Electrode (RRDE)



- RRDE system provides well-defined hydrodynamics for accurate reaction-convection-diffusion model
- IrO_x functionalized ring is a fast, robust pH sensor

Ideal for detecting local pH changes on planar electrodes

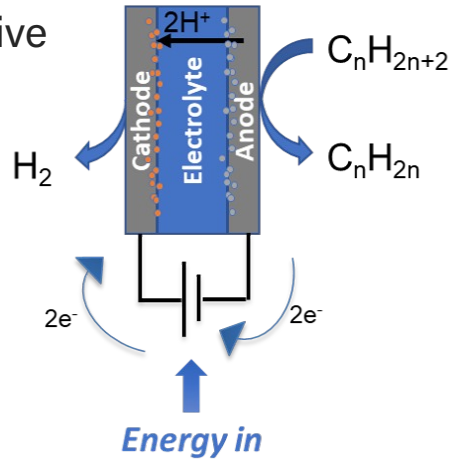
Why, What, and How?

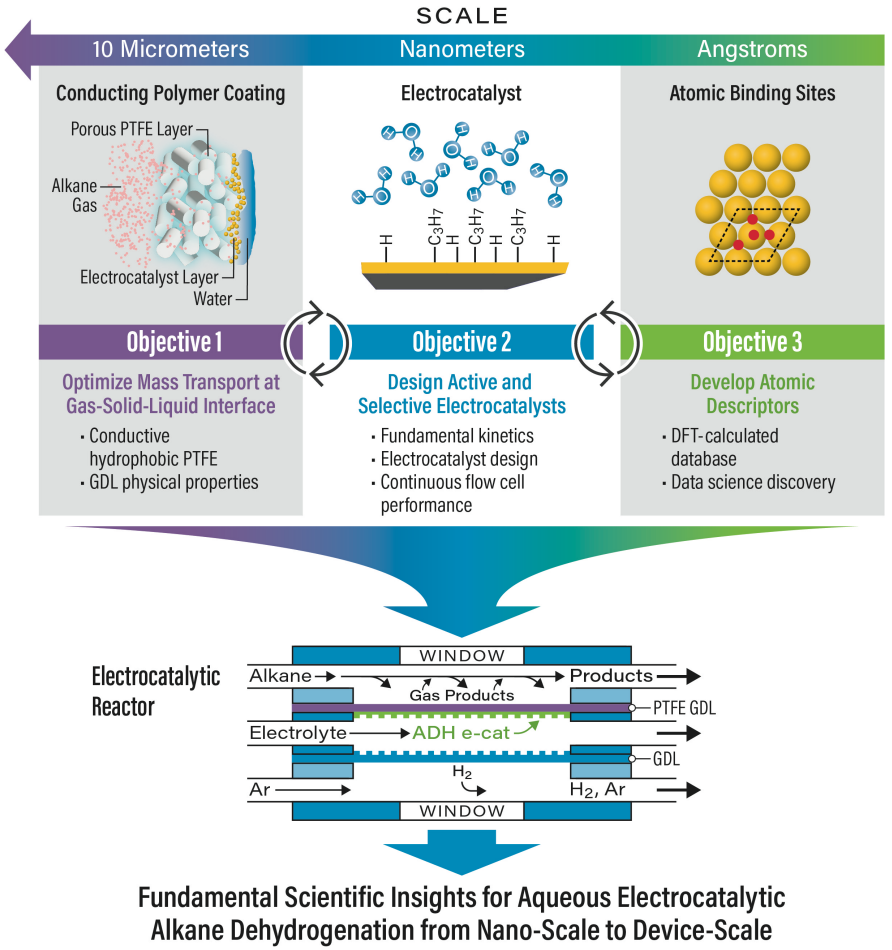
How Am I Approaching These Challenges?

- My lab has a unique combination of characterization techniques that enable study of a wide array of electron-driven chemical reactions

- Our department has collaborative and complementary faculty that enable multi-scale electrochemical reactor studies

  - Electrochemcial alkane dehydrogenation enhances safety → thermodynamic advantages of oxidative dehydrogenation without mixing O_2 + alkane.





Fundamental Scientific Insights for Aqueous Electrocatalytic Alkane Dehydrogenation from Nano-Scale to Device-Scale

Summary and Opportunities

- Electrochemical processes enable unique chemical manufacturing routes that could ***enhance process safety***
- Rapid influx of solar/wind ***motivates re-evaluation of electrochemical manufacturing***
- Realizing safe electrochemical process ***requires improvements in characterization/reactor configuration/education***
- My research approach is adaptable to broad range of electron driven chemistries that could ***improve safety of chemical manufacturing***

Potential opportunities to enhance safe chemical manufacturing with E-chem processes

- ***Propylene oxidation***
- ***Replace Cr-based reagents for C-H activation***
- ***Electrochemical H_2SO_4 synthesis***
- ***Electrochemical HNO_3 synthesis from air***
- ***Electrochemical Claus Process to treat industrial gases ($H_2S \rightarrow S$)***
- ***Indirect/mediated halogenations***