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Hydrogen Energy

Production and Utilization for a Green Economy

Alex Gupta

9/4/2020

Managed by Triad National Security, LLC for the U.S. Department of Energy's NNSA

About the Speaker

- Graduate Student, University of Louisville
  - Fall 2017 - Present
  - Mentor: Dr. Gautam Gupta
- Graduate Research Assistant, Los Alamos National Laboratory
  - January 2020 – Present
  - Mentors: Drs. Ulises Martinez, Rod Borup, Siddharth Komini-Babu, and Jacob Spendelow
- Research experience:
  - Electrocatalysis
  - Fuel cells
  - Corrosion
  - Materials science
  - Solar cells

Scope of this Presentation

1. Introduce high-level aspects of hydrogen fuel systems
2. Showcase research addressing relevant challenges
   - Proton exchange membrane fuel cells (PEMFCs)
     - Subzero temperature applications
     - AFM characterization of catalyst layers
   - Non-precious-metal hydrogen evolution catalysts

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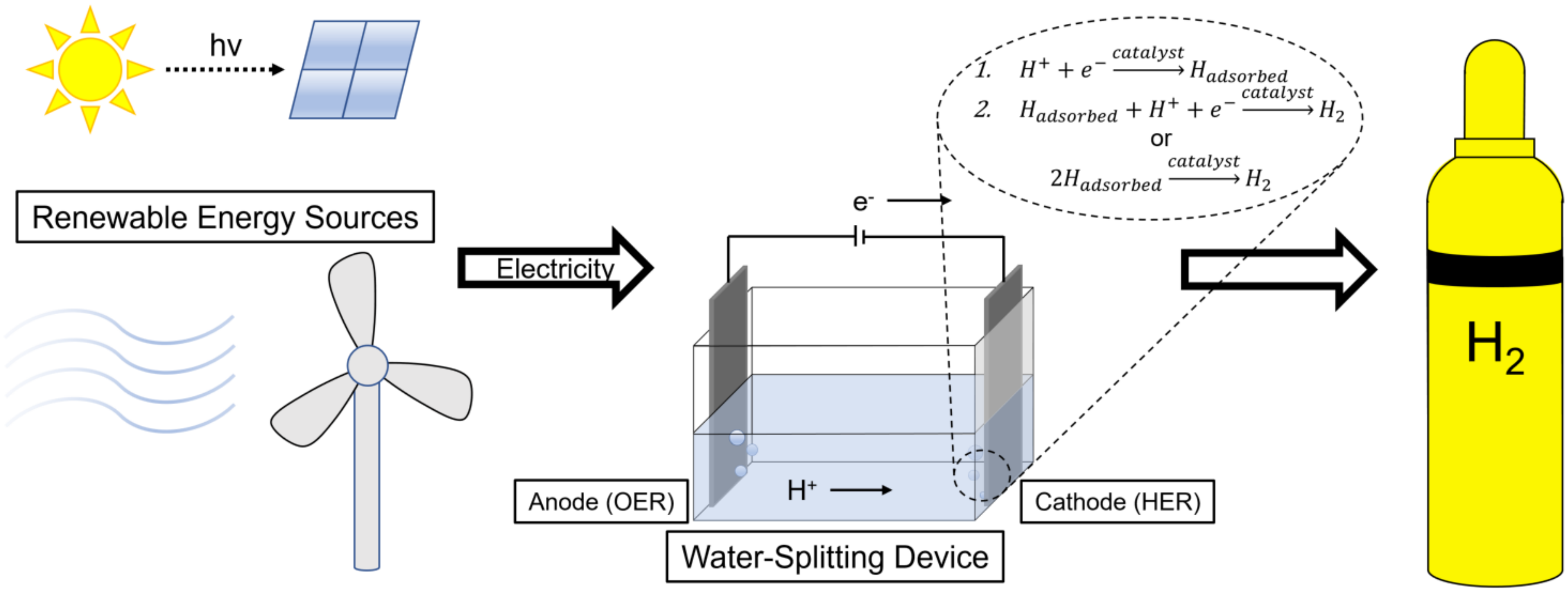
The Hydrogen Energy Landscape

Green Hydrogen Production

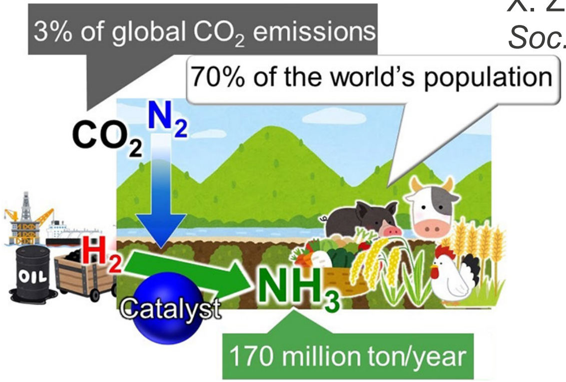


Hydrogen Applications

- Fossil fuel cracking/upgrading
- Ammonia production
- Hydrogenation
- **No-emission fuel cell electric vehicles**
  - Especially heavy duty (semi-trucks)
  - H_2 from steam reformation less suitable

X. Zou, Y. Zhang, *Chem. Soc. Rev*. **44**, 5148 (2015).

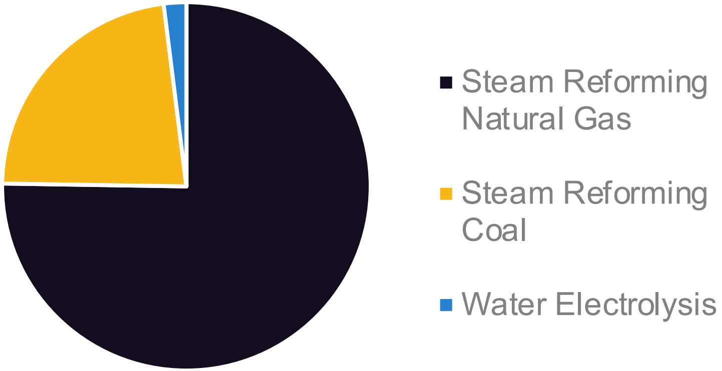
Toyota

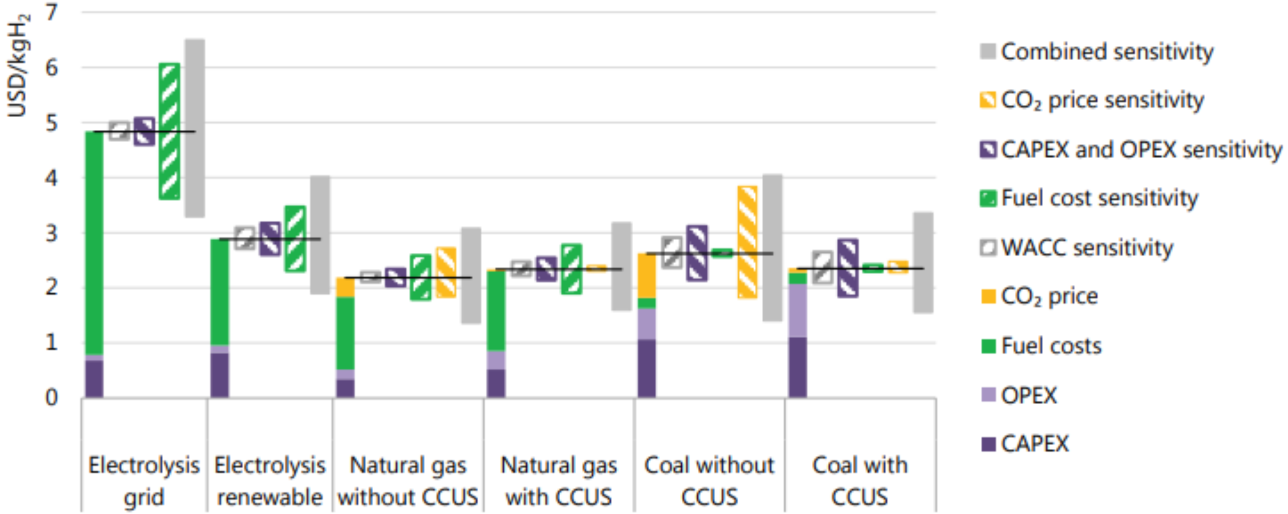


azocleantech.com

Current Status

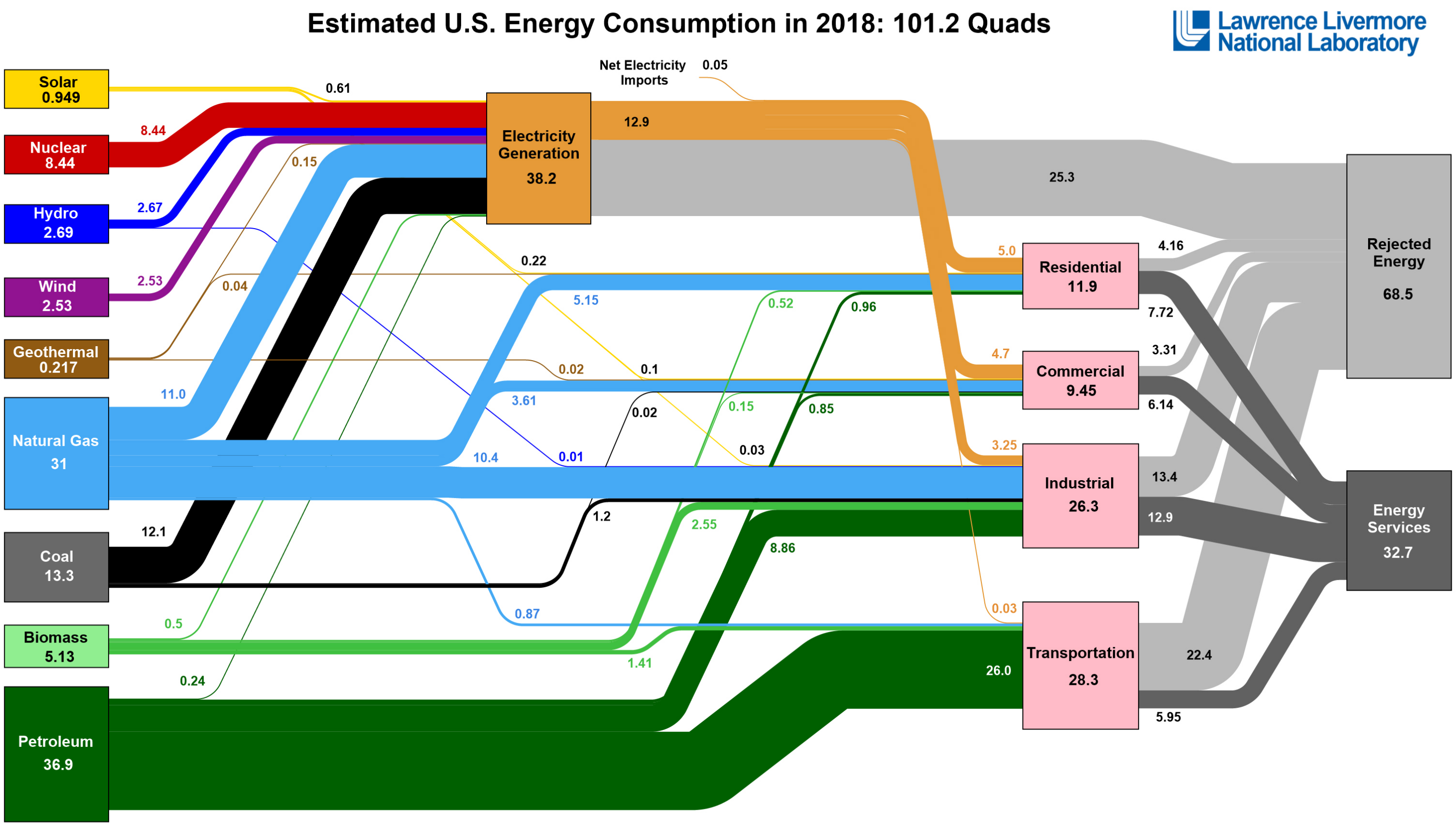
- Hydrogen produced mainly by steam reforming
  - 2 % from water electrolysis
    - Primarily due to cost



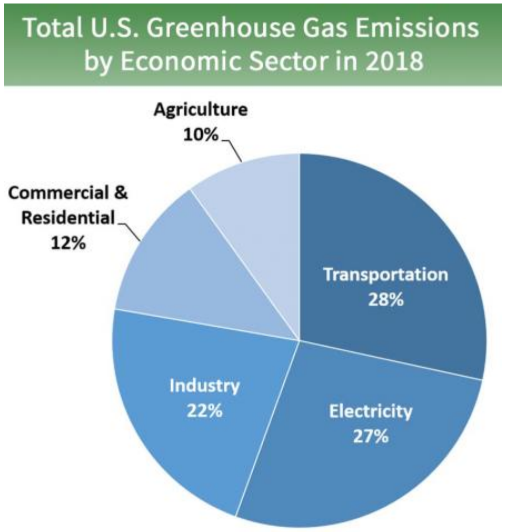


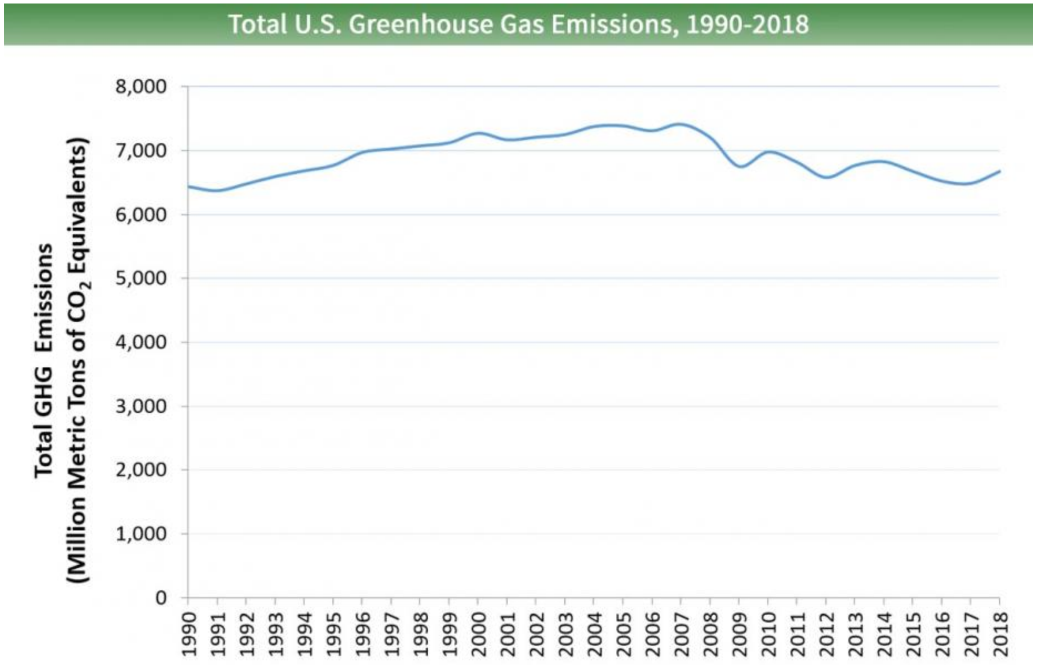
IEA, "The Future of Hydrogen" (2019).

Energy Consumption



Greenhouse Gas Emissions



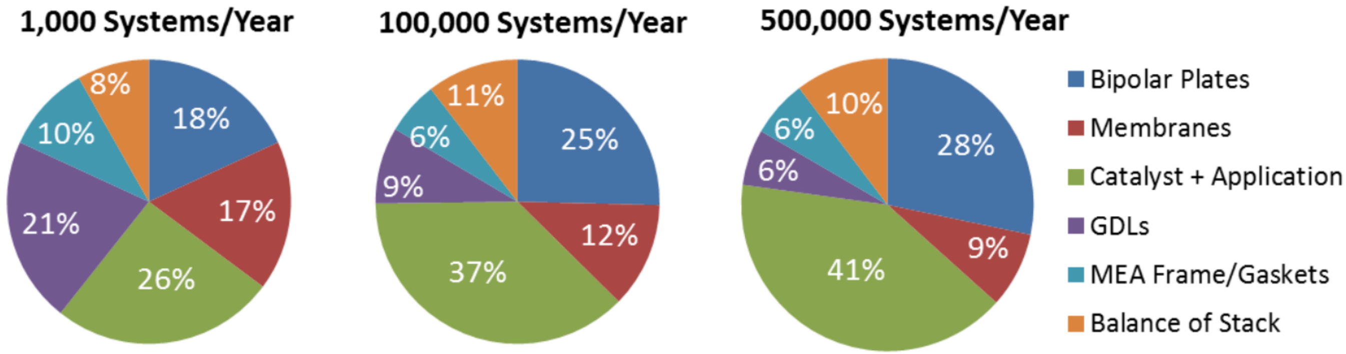


Using green hydrogen to fuel even part of the economy would drastically reduce greenhouse gas emissions

United States Environmental Protection Agency

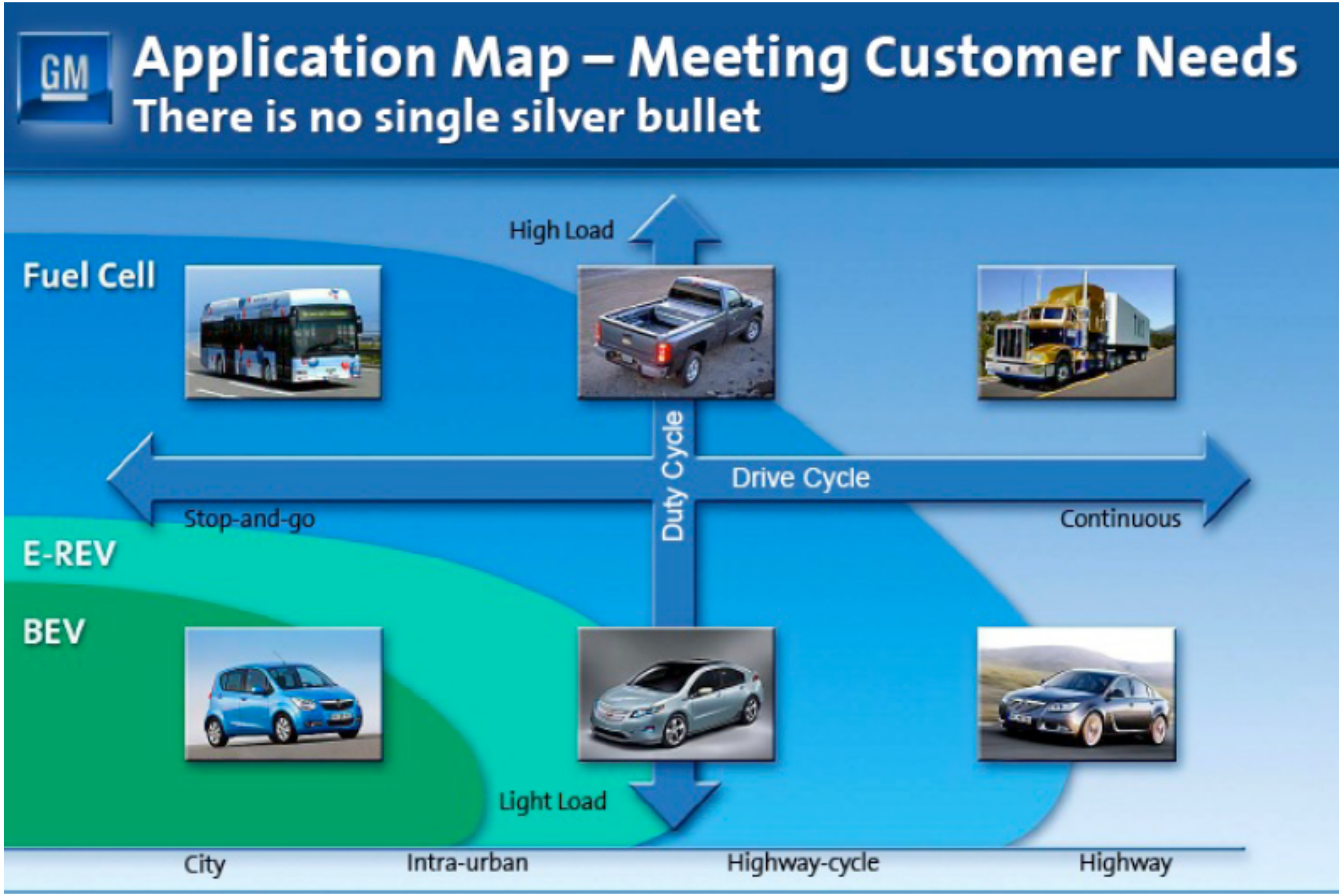
PEM Electrolyzer & Fuel Cell Cost Challenge

- Approaches:
  - Reduce precious metal content
  - Improve catalyst performance
  - Design electrodes to utilize more of the catalyst
  - Make more durable devices
  - Replace catalysts with non-precious metals
- Other challenges:
  - Hydrogen storage & distribution
  - Device durability
  - Competition with existing technologies
  - Efficacy of renewable energy sources
  - System efficiency (balance of plant)



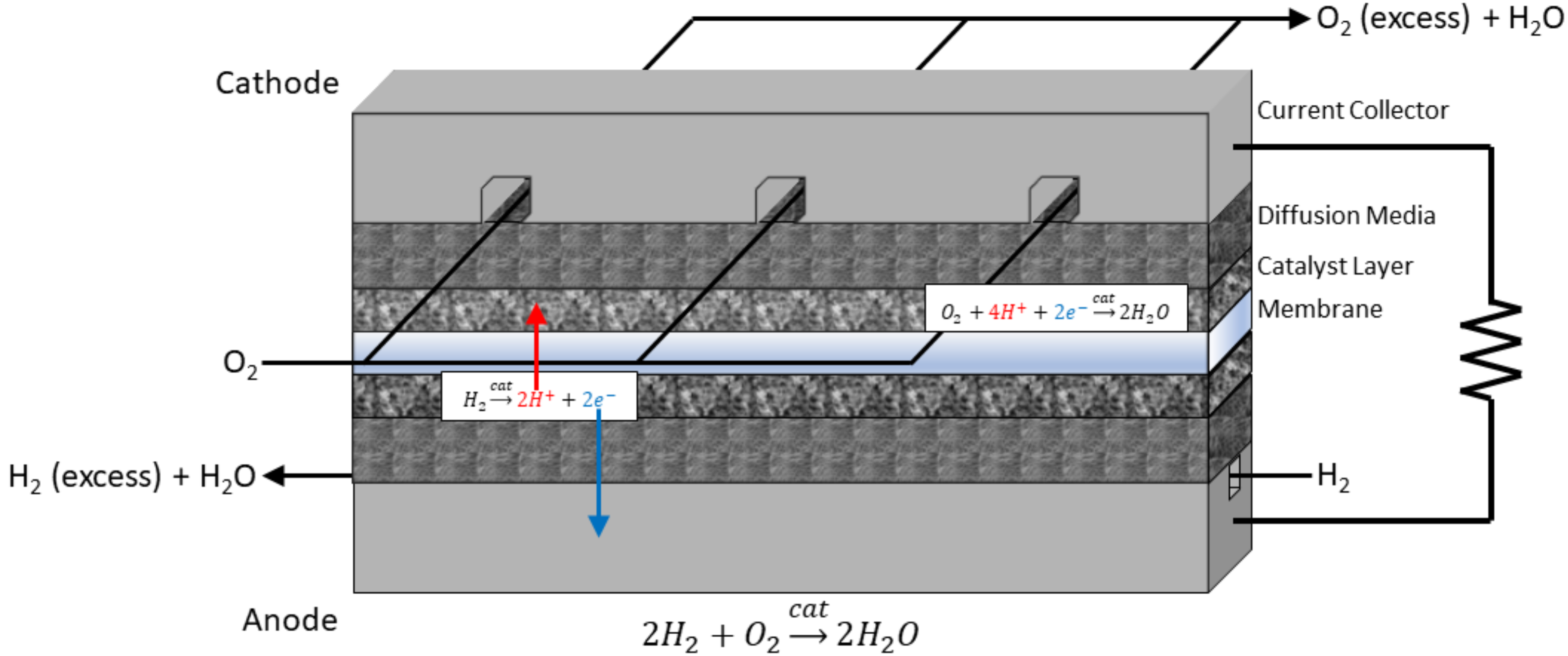
A. Wilson *et al.*, “DOE Hydrogen and Fuel Cells Program Record Title: Fuel Cell System Cost-2017 Originator” (2017).

Why Hydrogen?

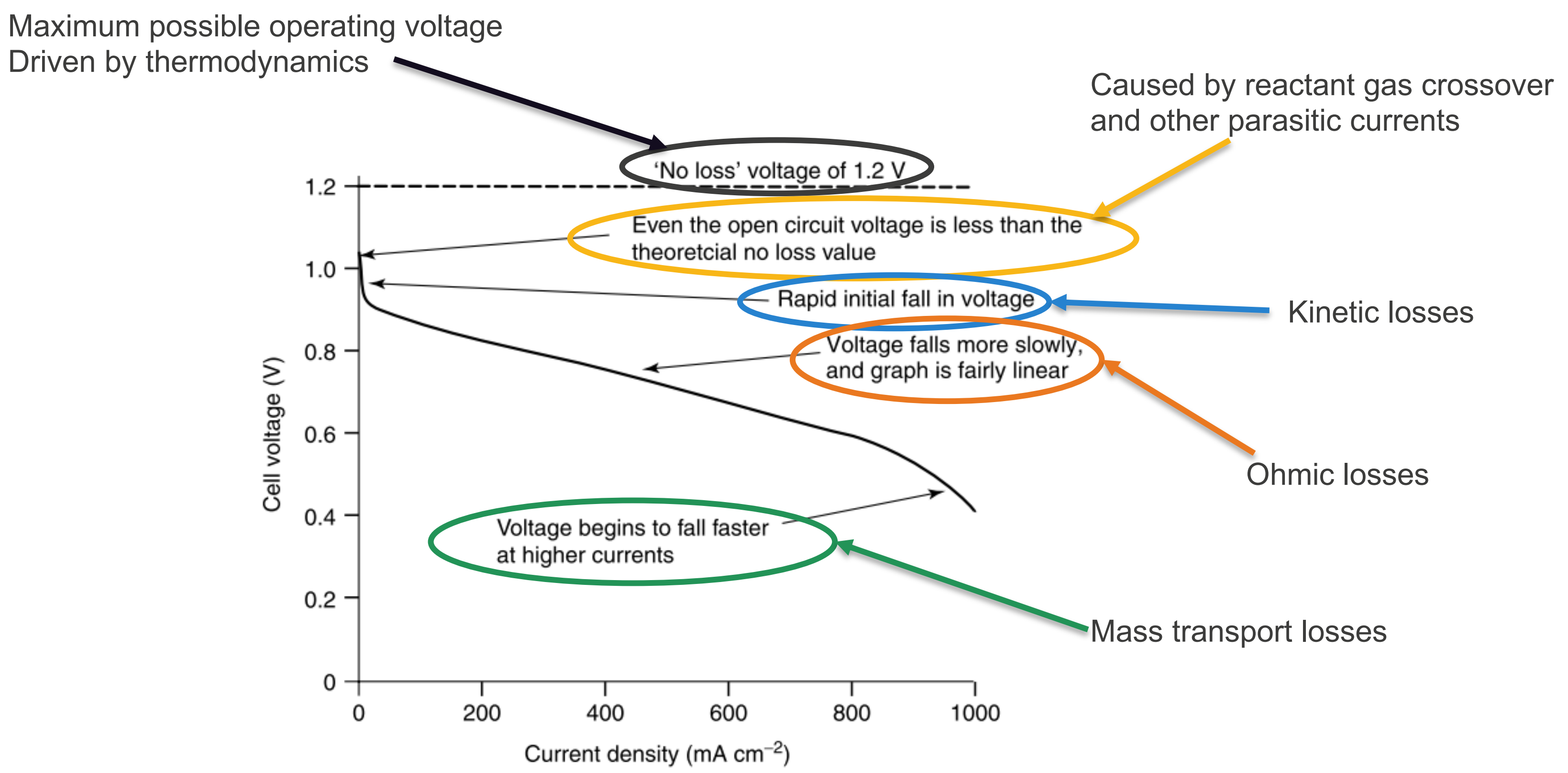


Proton Exchange Membrane Fuel Cells

Anatomy of a Fuel Cell

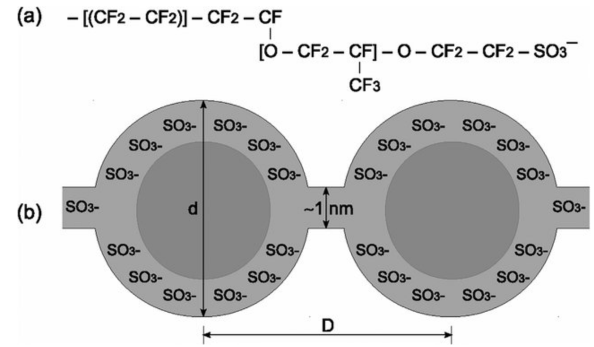


Fuel Cell Polarization Curve

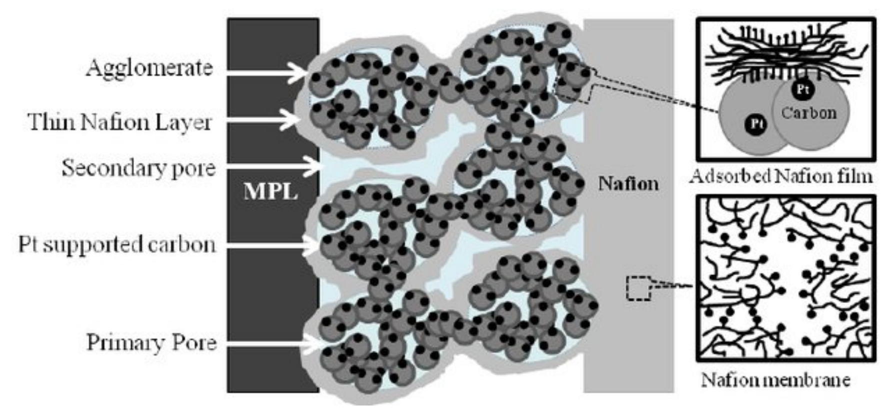


Fuel Cells Component Breakdown

- Membrane:
  - Hydrophilic channels
  - Hydrophobic PTFE backbone
- Catalyst layer:
  - Pt: Catalyzes reaction
  - C: Electrically conductive support
  - Ionomer: Conducts protons to active sites
- Diffusion media:
  - Microporous layer
  - Gas diffusion layer
- Each component affects the performance!



H. E. Andrada et al, *Int. J. Hydrogen Energy*. **43**, 8936–8943 (2018).

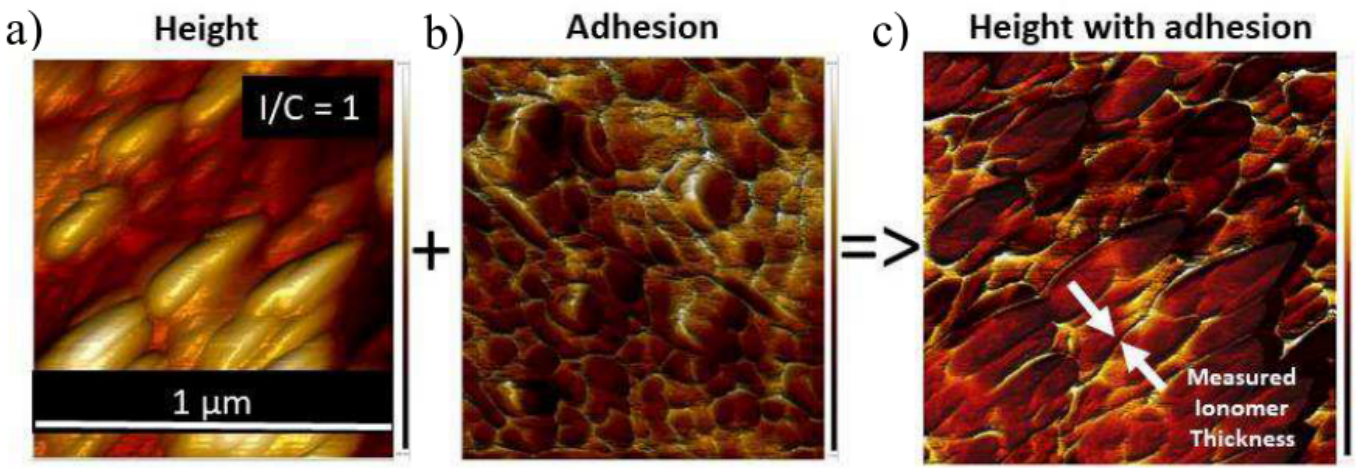


D. Paul et,al *ECS Trans.* **41**, 1393–1406 (2019).

Fuel Cell Experiments at LANL

AFM Analysis of PEMFC Catalyst Layers

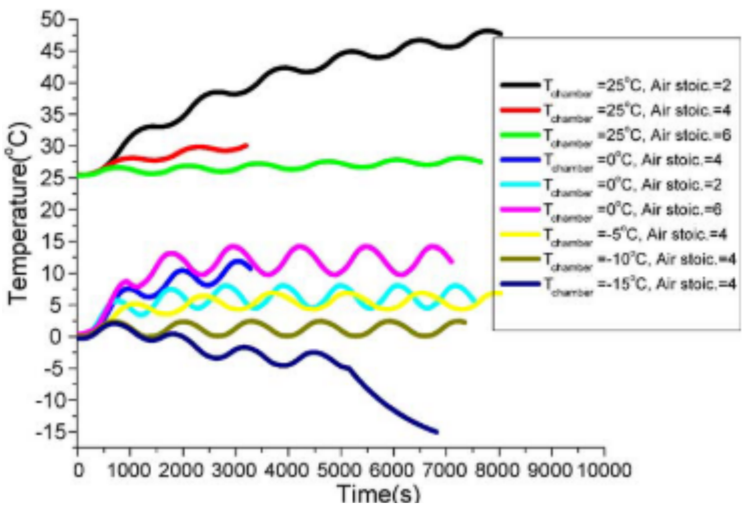
- Positive correlation between ionomer content and agglomerate size directly identified
- Currently working to combine quantitative nanomechanical mapping with tunneling microscopy
  - Direct correlation/comparison of electrical, mechanical, and morphological features.
- Goal: Correlate nanoscale features with performance and use the information to design more durable cells

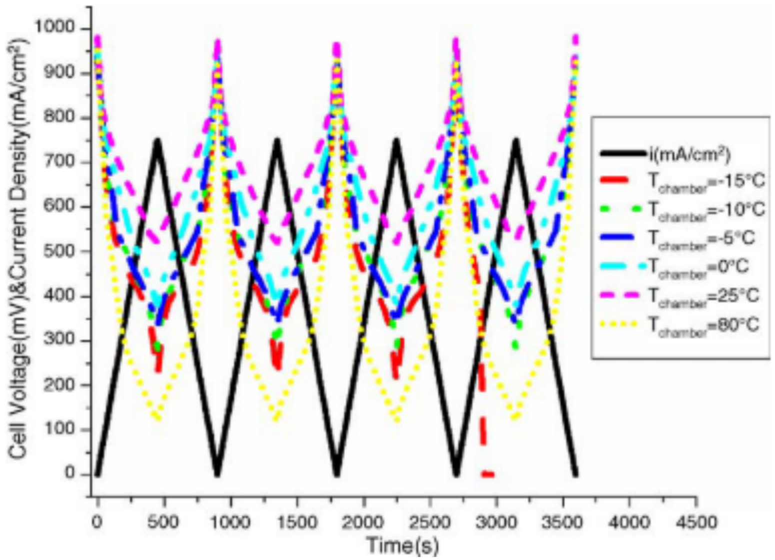


K. Chintam *et al.*, *ECS Trans.* **92**, 95–105 (2019).

Fuel Cell Operation at Subzero Temperature: Background

- Below ~-15 °C, reaction heat is insufficient to raise device temperature above 0 °C
- Accumulation of enough ice causes device failure

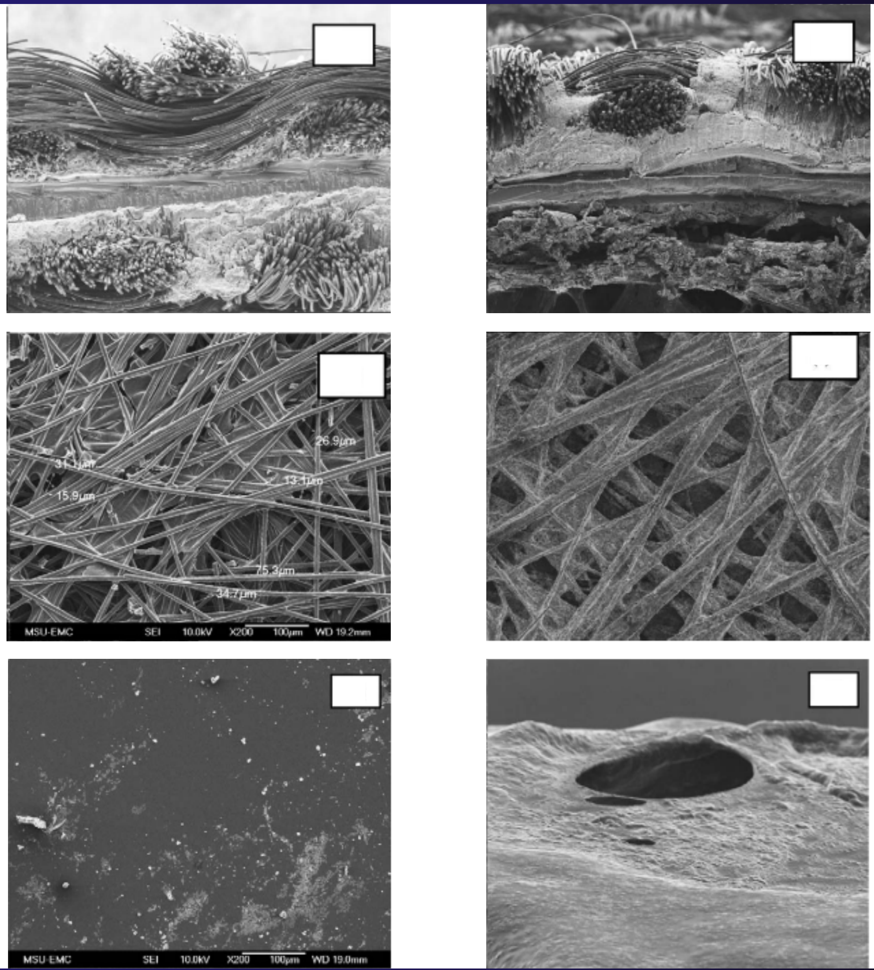




Q. Yan, H. Toghiani, Y. W. Lee, K. Liang, H. Causey, *J. Power Sources*. **160**, 1242–1250 (2006).

Fuel Cell Operation at Subzero Temperature: Background

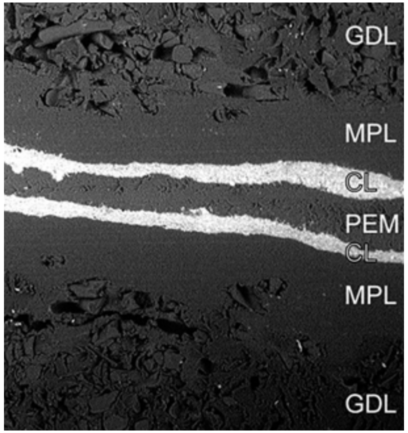
- Effects of freezing:
  - Blocking of active sites / reactant gas diffusion pathways
  - Delamination of CL from membrane and/or DM
  - Fraying & swelling of carbon fibers in DM (water penetration, coating delamination)
  - Membrane damage
    - Roughened surface, cracking, pinholes promoting crossover
- Ice buildup must be avoided!

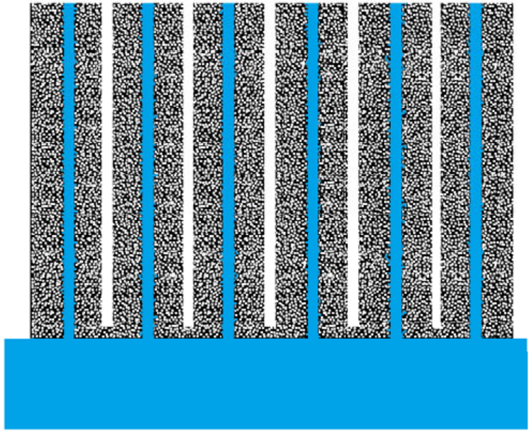


Q. Yan, H. Toghiani, Y. W. Lee, K. Liang, H. Causey, *J. Power Sources*. **160**, 1242–1250 (2006).

Fuel Cell Operation at Subzero Temperature: Our Approach

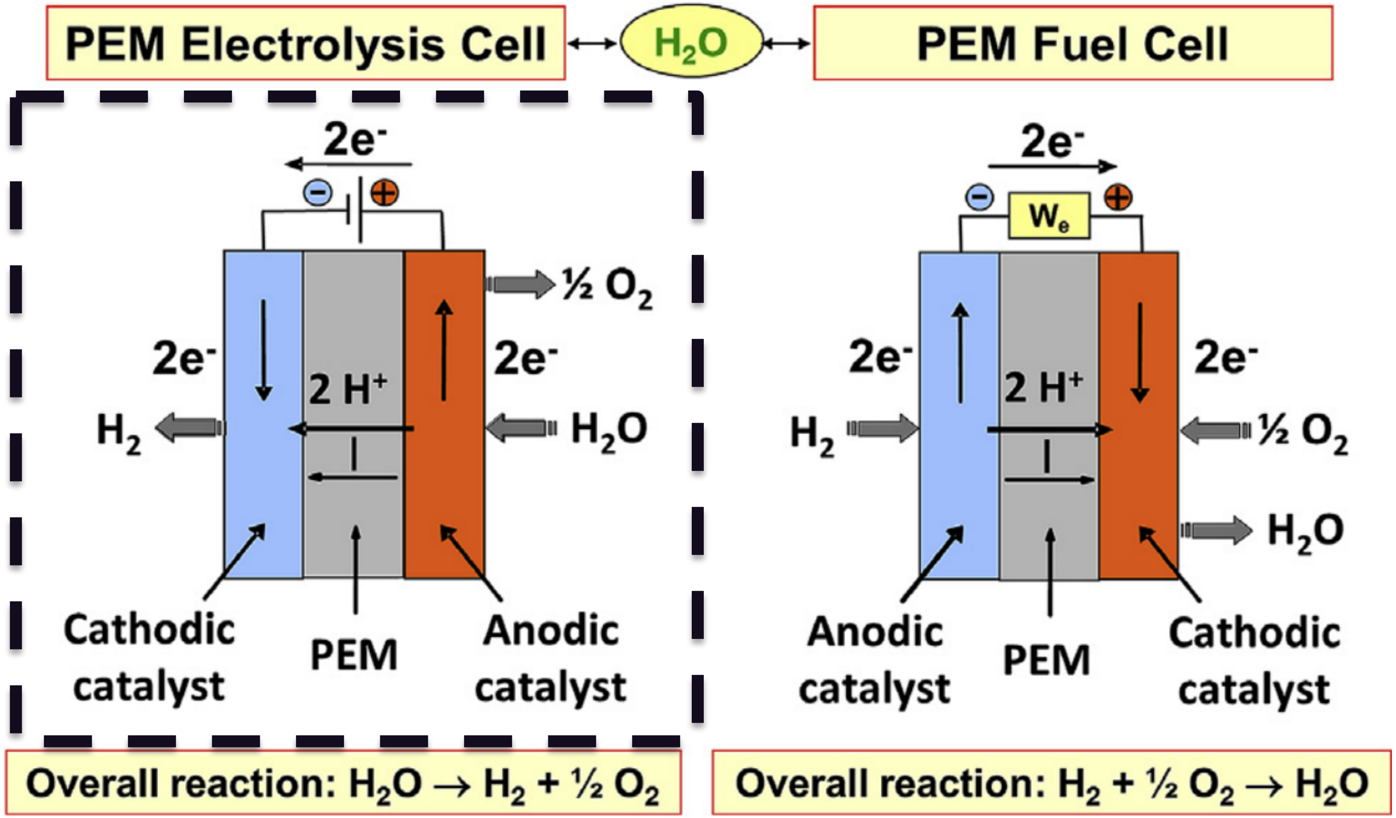
- Address problems by component:
  - Diffusion media (DM)
    - Keep water out
  - Catalyst layer (CL)
    - Move water out quickly before it accumulates
  - Membrane
    - Use as a reservoir for product water
    - Use dopants to attenuate freezing water content
- Use structured components to:
  - Confer hydrophobicity to DM and CL
  - Facilitate water transport to membrane
    - Shorter distance
  - Optimize both activity and stability





PEM Electrolyzers

Electrolyzer vs. Fuel Cell



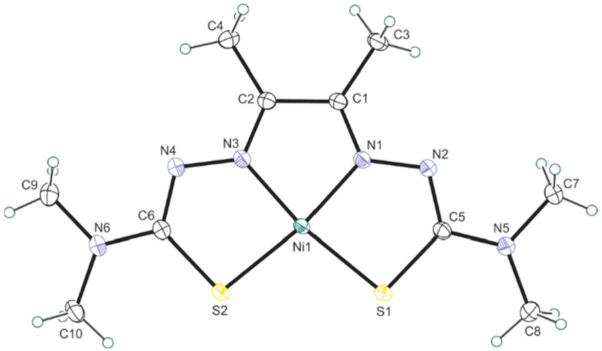
C. Lamy, *Int. J. Hydrogen Energy*. **41**, 15415–15425 (2016).

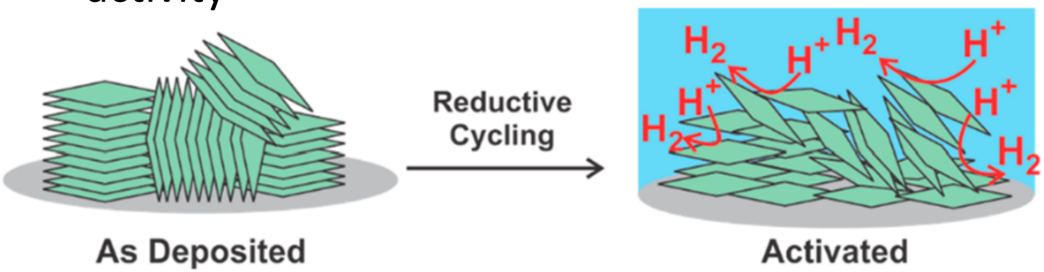
Non-Precious-Metal Catalysts for Hydrogen Evolution

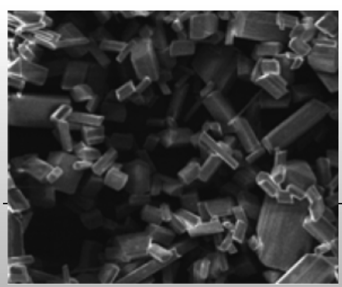
Work Performed at U of L

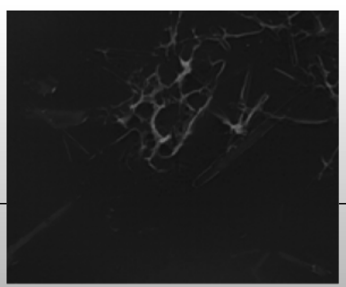
Bis-thiosemicarbazone Catalysts for HER

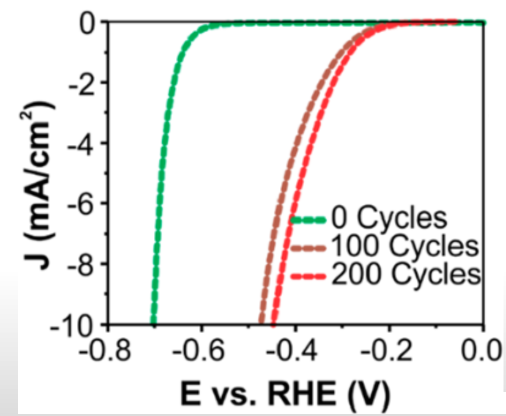
- Initially poor catalytic activity
  - Bigger current @ lower voltage = better
- Activity improves by cycling the catalyst
  - Dynamic rearrangement
- Ligand substitution affects resulting catalytic activity







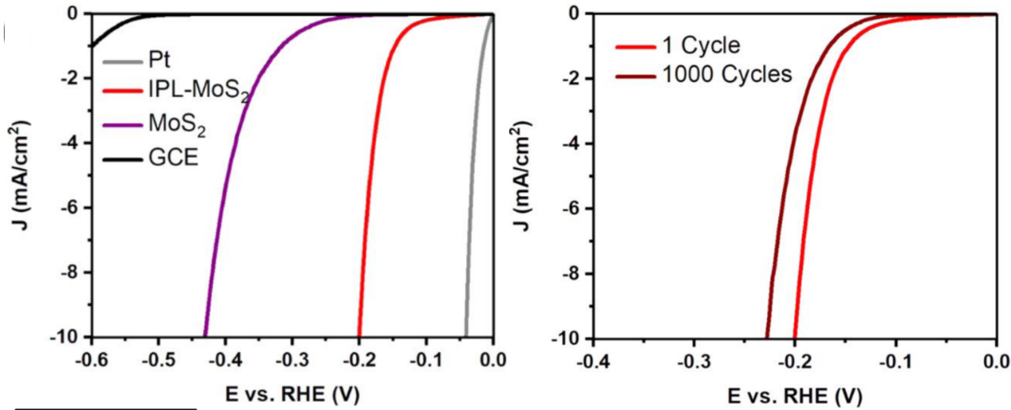


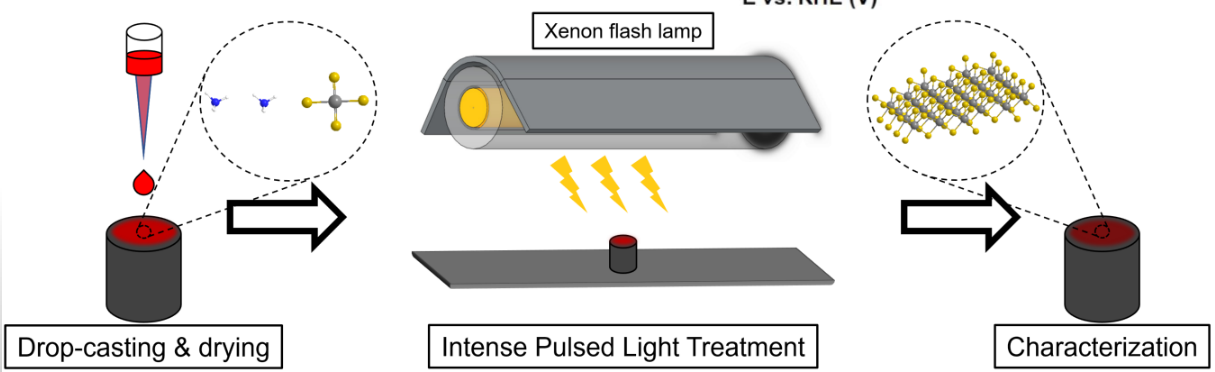


A. J. Gupta *et al., Inorg. Chem.* **58**, 12025–12039 (2019).

Transition Metal Chalcogenide Catalysts for HER

- Precursor converted to MoS_2 directly on substrate by photon energy
- Resulting material:
  - Has good stability
  - Shows activity comparable to other highly-active MoS2 catalyst preparations





A. Gupta *et al.*, *Nanotechnology*. **30** (2019)

Outlook

- The possibilities are endless for applications of electrochemical hydrogen systems and routes to the eventual realization of the hydrogen economy.

- *"If the fuel cell is to become the modern steam engine, basic research must provide breakthroughs in understanding, materials, and design to make a hydrogen-based energy system a vibrant and competitive force."*

  – G. W. Crabtree et al, *Phys. Today*. **57**, 39–44 (2004).

Acknowledgements

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