U.S. DEPARTMENT OF ENERGY | Office of Science

BES Virtual Roundtable on "Foundational Science for Carbon Neutral Hydrogen Technologies" August 2-5, 2021

Co-Chair: Morris Bullock
Pacific Northwest National Laboratory

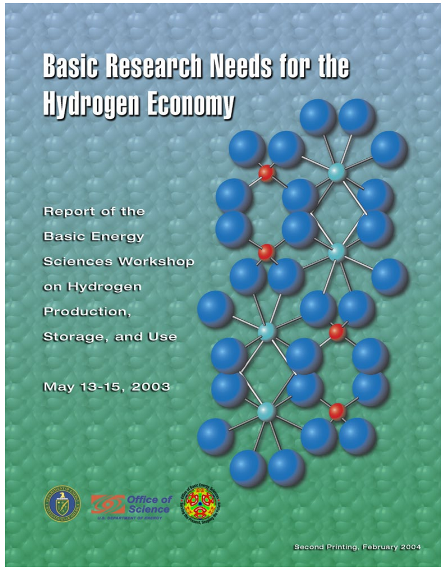
Co-Chair: Karren More
Oak Ridge National Laboratory

Briefing to the Basic Energy Sciences Advisory Committee

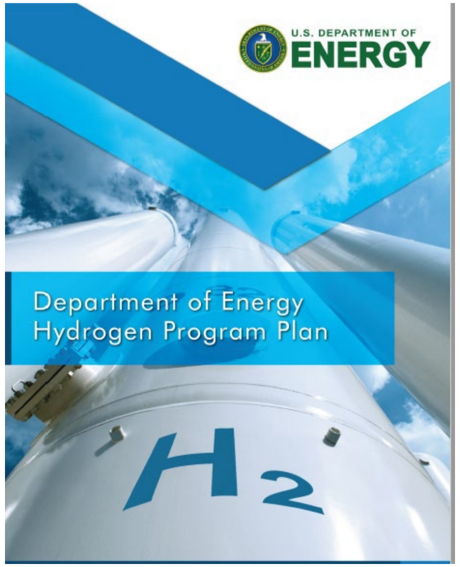
December 6, 2021

Previous DOE Reports

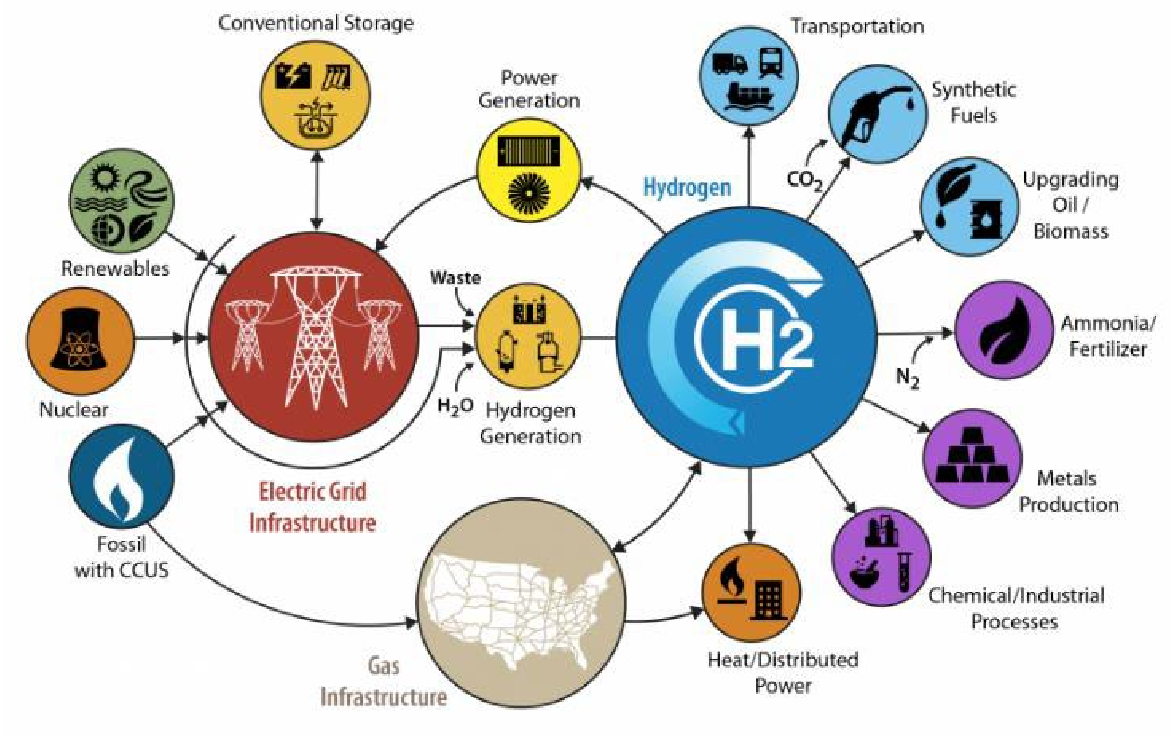
- BES-Basic Research Needs for the Hydrogen Economy
  "BES Workshop on Hydrogen Production, Storage, and Use"
  May 13-15, 2003
  M. Dresselhaus (MIT), George Crabtree (ANL),
  Michelle Buchanan (ORNL



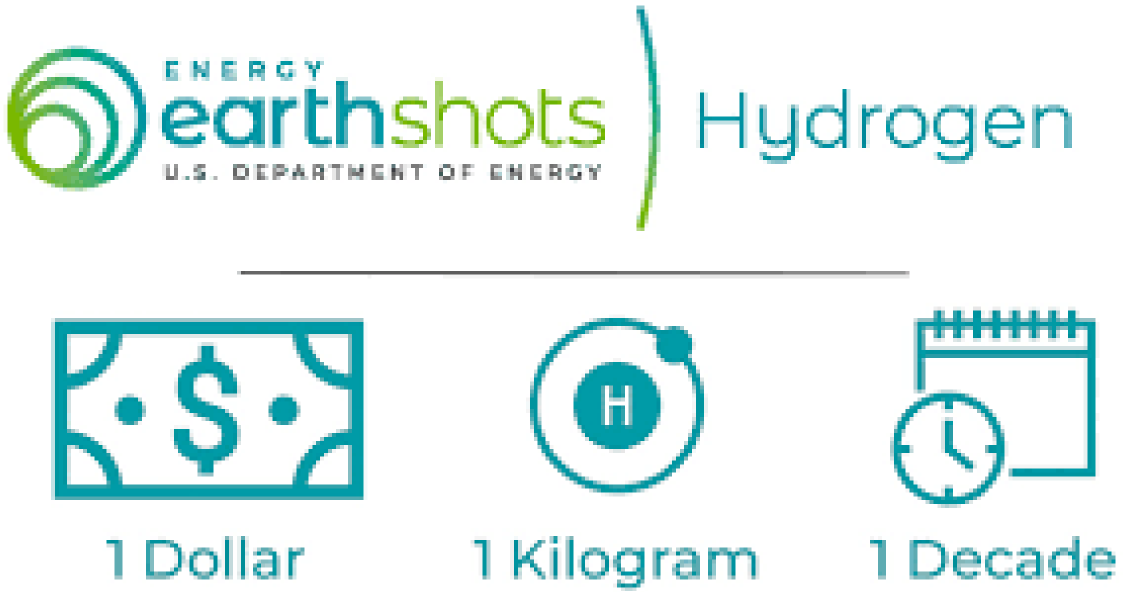
- US DOE Hydrogen Program Plan – a coordinated high-level summary of hydrogen-related activities across DOE offices (Energy Efficiency and Renewable Energy, Fossil Energy, Nuclear Energy, electricity, Science, and ARPA-E) - reflects DOE's focus on coordinating R&D efforts to enable the adoption of hydrogen technologies across multiple sectors – November 2020



"Hydrogen" is central to DOE's clean energy strategy



H2@Scale



Hydrogen Shot "1 1 1"

Virtual Roundtable Charge

Co-chairs: Morris Bullock (PNNL)
Karren More (ORNL)

Date: Virtual, August 2-5, 2021

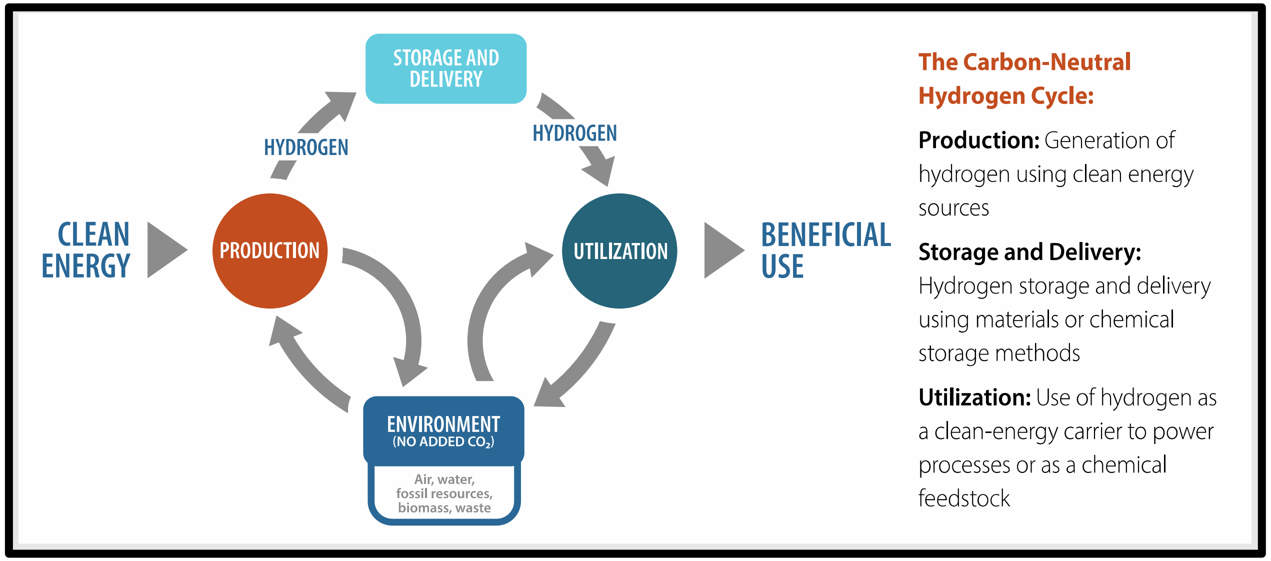
Virtual Roundtable led by SC-BES

With participation by:

- EERE Hydrogen & Fuel Cells Technology Office (HFTO)
- Fossil Energy and Carbon Management (FECM)
- Nuclear Energy (NE)

Charge:

- Discuss scientific and technical barriers associated with carbon-neutral hydrogen *production*, *storage*, and *utilization*
- Identify Priority Research Opportunities (PROs) for fundamental science that will accelerate progress toward energy-efficient, carbon-neutral cycles for hydrogen processes
- PROs will describe the most important research directions that will form the basis for a coordinated, long-term strategy and provide guidance to the research community over the next decade



Roundtable Panels

- Hydrogen **Production**
  - Panel Lead – Jingguang Chen, Columbia University

- Hydrogen **Storage**
  - Panel Lead – Krista Walton, Georgia Institute of Technology

- Hydrogen **Utilization**
  - Panel Lead – Bryan Pivovar, NREL

- **Cross-Cutting**
  - Panel Co-Leads – Aleksandra Vojvodic, University of Pennsylvania
    – Daniel Resasco, University of Oklahoma

Roundtable participants represented Universities (18), Industry (2), and National Laboratories (6)

Roundtable – Plenary Speakers

Challenges of Large-Scale Water Electrolysis and Implications for Advanced Water Splitting Technologies

Kathy Ayers
Nel Hydrogen

Cavendish + 255: What's Next for H_2 Science?

Tom Baker
University of Ottawa

Challenges and Opportunities for Hydrogen Utilization

Levi Thompson
University of Delaware

Path to define Priority Research Opportunities (PROs)

Day 1

H_2 Production	H_2 Storage	H_2 Utilization	Cross-cutting
Directed Design of Electrolysis Materials	Design and understand materials and catalysts with desired H_2 binding energetics & selectivities	Science of stability/degradation	Develop integrated theoretical/experimental approach/framework to understand and control complex phases and interfaces
H_2 from hydrocarbons and biomass	Advanced computational and experimental techniques	Persistent changes of materials and interfaces	In situ elucidation of electrochemical interfaces
		H_2 transformations through coupled micro-environments and processes	

Co-Chairs, Panel Leads, and DOE: refine and consolidate candidate PRO topics from Day 1 into four PROs for further development on Day 2

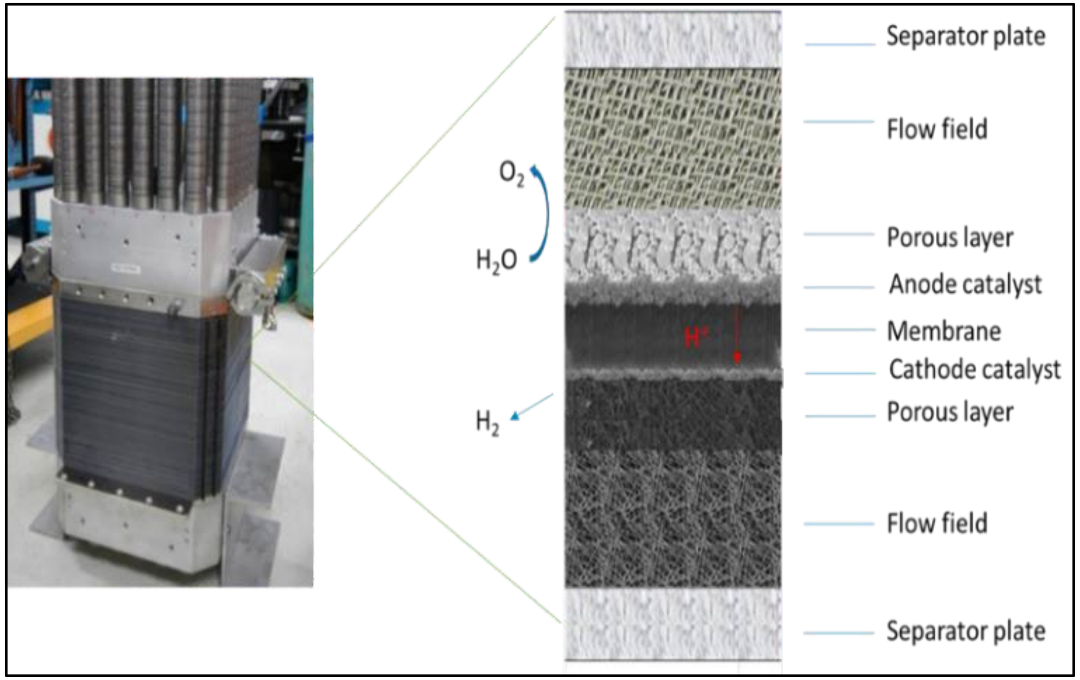
Day 2

PRO 1 Electrolysis PL: Jingguang Chen	PRO 2 H_2 interactions PL: Krista Walton	PRO 3 Interfaces PLs: Dan & Aleks	PRO 4 Degradation PL: Bryan Pivovar
• Tailored for different environment • Improved/novel materials synthesis • Alkaline, PEM, HT • Capabilities or approaches needed	• Storage • H_2 reactions • Binding energetics • Embrittlement • Capabilities or approaches needed	• interface complexity • Understand, tune, control temporal and spatial phenomena • Capabilities or approaches needed	• Dynamic evolution • Operando studies • Improved materials stability • Capabilities or approaches needed

Panelists re-aligned to finalize four PROs

PRO 1: Discover and Control Materials and Chemical Processes to Revolutionize Electrolysis Systems

- ***Key question:*** *How do we codesign multiple components that work together to enable stable, efficient electrolysis for carbon-free production of hydrogen from water?*
- Electrolysis requires the coordinated actions of many components under specific operating conditions to achieve high activity and tolerance to impurities in water. To make significant advances, it is critical to achieve a detailed mechanistic understanding of how the materials components, systems, and reaction environment work together to produce hydrogen. Understanding multiscale temporal and spatial phenomena is essential for the directed codesign of cost-effective, stable components, including catalysts, membranes, and electrode layers for different operating environments. Toward these goals, the development of in situ and/or operando characterization techniques and computational and/or data science tools is needed to capture the evolving complexity of systems under working conditions.



Components of a PEM electrolyzer cell and stack.

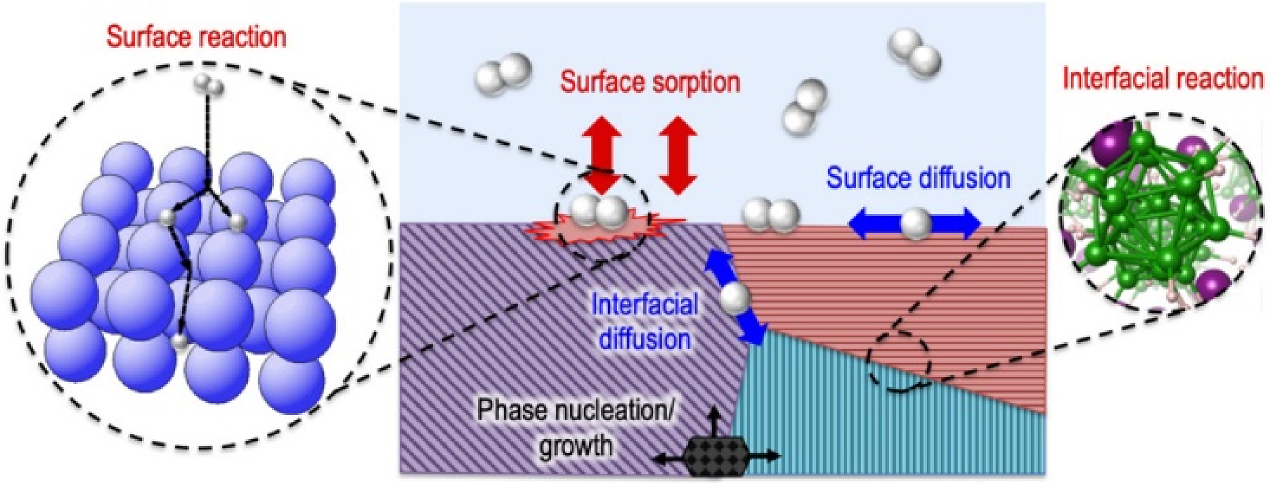
Villagra, et al., *International Journal of Hydrogen Energy* **44** (2019).

PRO 2: Manipulate Hydrogen Interactions to Harness the Full Potential of Hydrogen as a Fuel

- ***Key question:*** *What fundamental insights are needed to control and selectively tune hydrogen interactions with molecules and materials?*
- Successful carbon-neutral hydrogen technologies require controlling the energetics and mechanisms of hydrogen interactions with molecules and materials. The range of energies that must be controlled spans from weak hydrogen interactions to the strong bond in molecular H_2. Gaining the ability to tune hydrogen interactions for specific binding energies that are stronger than physisorption yet weaker than chemisorption will provide a transformative advance in hydrogen technologies. Mastering this control will require the ability to characterize hydrogen interactions and dynamics for storage and utilization processes at surfaces and interfaces, in molecular species and confined environments, and in integrating these data into predictive models.

Schematic of some of the key surface and interface processes taking place during cycling of a typical nanoscale metal hydride material.

B.C. Wood, et al., *Industrial & Engineering Chemistry Research* **59** (2020).

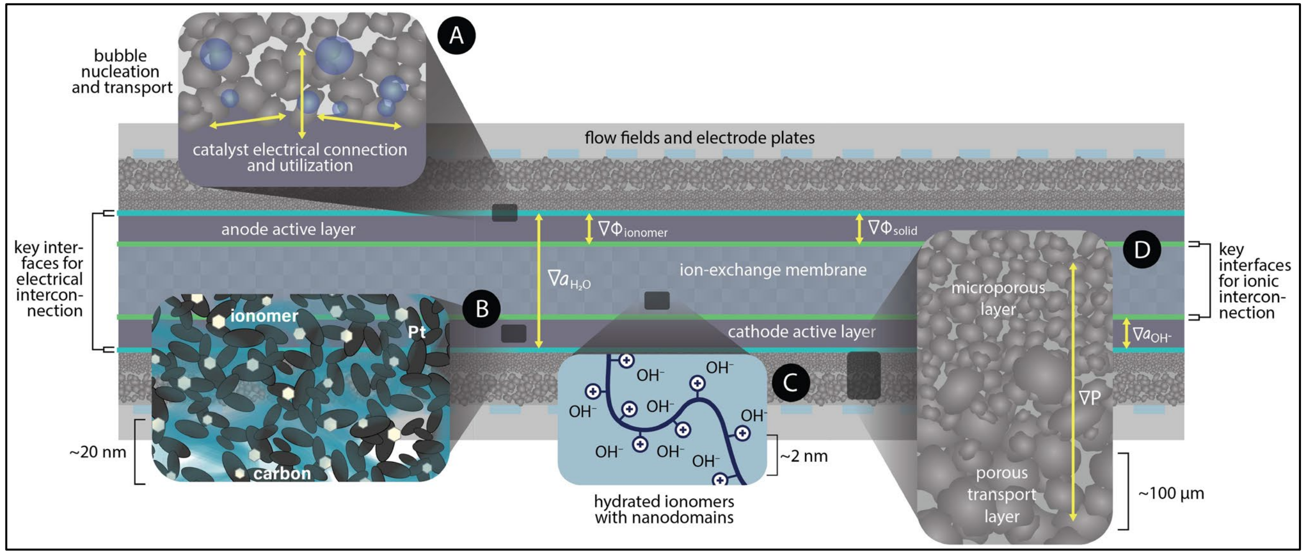


PRO 3: Elucidate the Structure, Evolution, and Chemistry of Complex Interfaces for Energy- and Atom-Efficiency

- ***Key question:*** *How can interacting, evolving interfaces be tailored at multiple length scales and timescales to achieve energy-efficient, selective processes and enable carbon-neutral hydrogen technologies?*

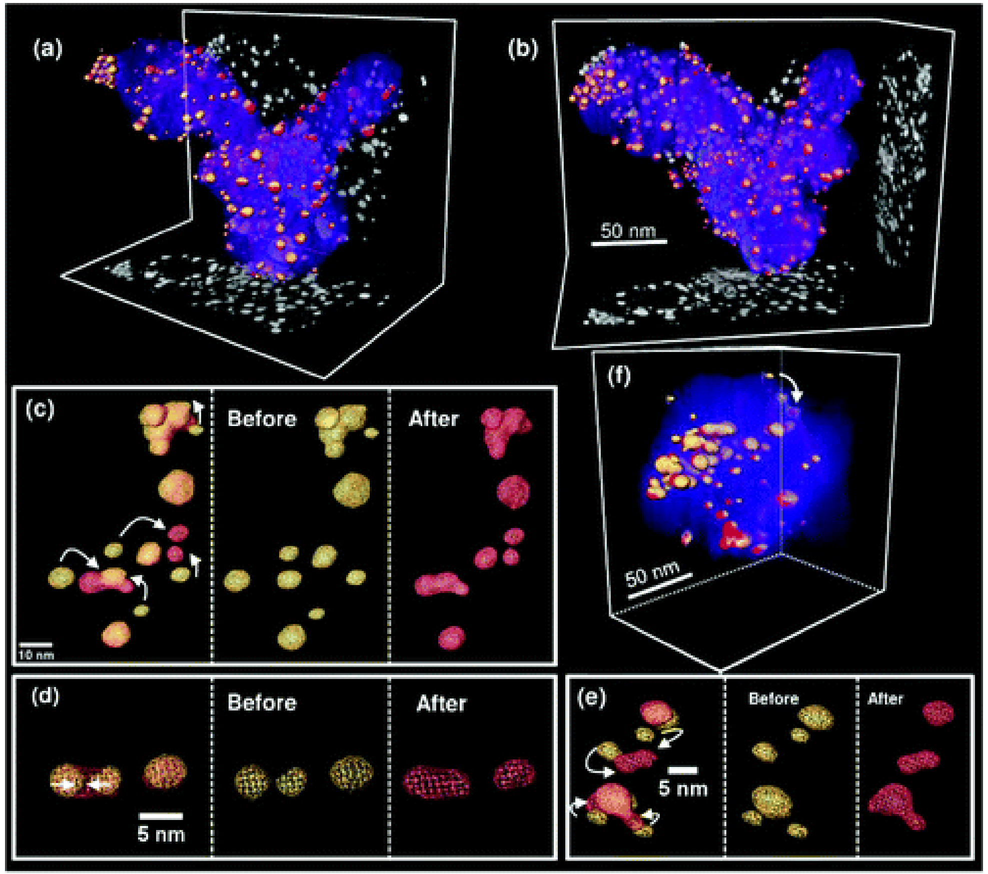
- The complexity of the many multicomponent, multiphase interfaces coupled with the reactivity inherent in hydrogen systems present many challenges. Achieving sustainable processes requires atom-efficient chemical reactions that do not waste atoms or create unwanted by-products. Mapping, understanding, and controlling the spatiotemporal properties and dynamics of complex interfaces involving multiple phases is key to advancing carbon-neutral hydrogen technologies. This major challenge requires the development of integrated, predictive approaches that involve the coupling and parallel application of diverse techniques, including advanced synthesis; ex situ, in situ, and operando characterization; theoretical understanding and modeling from quantum to continuum length scales; data science and machine learning; performance measurements; and multimodal platforms to couple these methods.

Schematic illustration of critical component materials, three-dimensional architectures, and interfaces in an example membrane electrolyzer. Key driving forces leading to bulk and interface reaction and transport processes are shown.



PRO 4: Understand and Limit Degradation Processes to Enhance the Durability of Hydrogen Systems

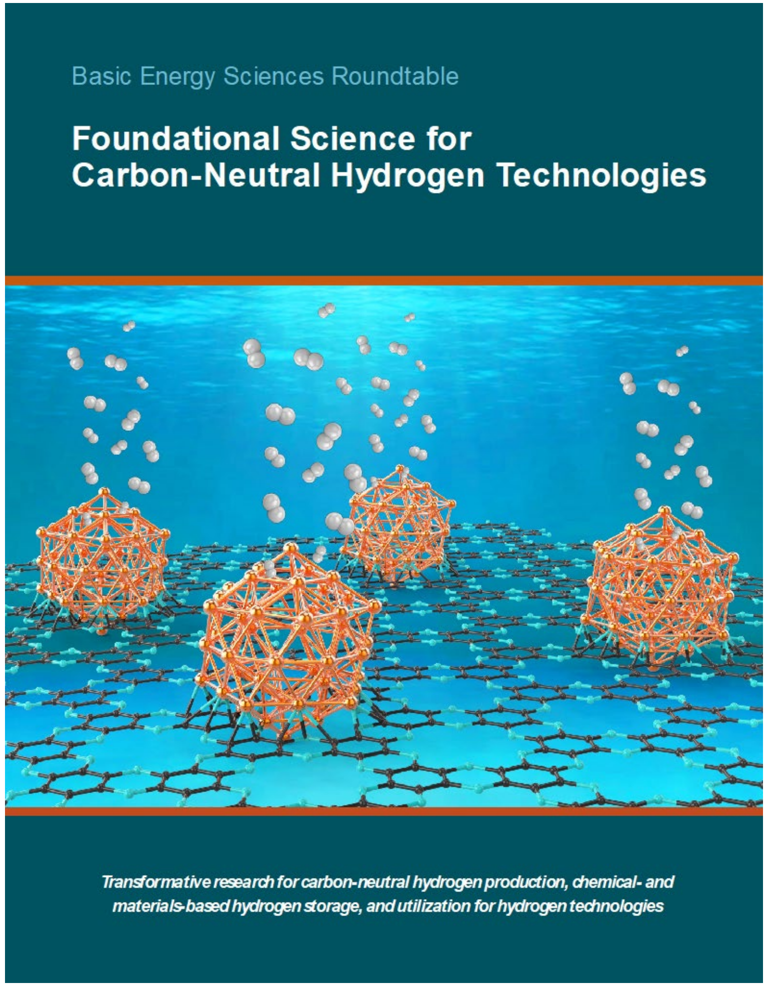
- ***Key question:*** *How can we identify and understand the complex mechanisms of degradation to obtain foundational knowledge that enables the predictive design of robust hydrogen systems?*
- Understanding and mitigating degradation is a formidable challenge in many hydrogen technologies. The lack of mechanistic understanding of multiple degradation phenomena at a molecular or atomic scale is exacerbated by their occurrence over long time periods and the complexity of operating environments. Recognizing the structure-function relationships that govern stability is essential, including performing operando process characterization at interfaces. Such understanding will lead to new design principles and result in more robust, stable materials with significantly enhanced lifetimes, especially when synthesis and performance are coupled with predictive modeling.



One-to-one correspondence of nanocatalyst particles before (gold) and after (red) electrochemical aging using electron tomography.

Yu, et al., *Nano Letters* **12** (2012).

Status of Outcomes

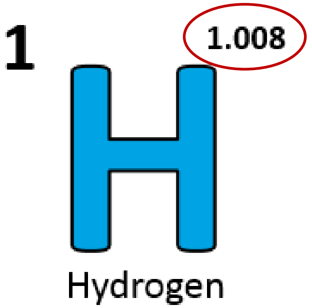

Basic Energy Sciences Roundtable

Foundational Science for Carbon-Neutral Hydrogen Technologies

Transformative research for carbon-neutral hydrogen production, chemical- and materials-based hydrogen storage, and utilization for hydrogen technologies

Technology Status Document

Debbie Myers
Argonne National Lab



Roundtable Brochure
and
Technology Status Document
posted on BES website
October 8, 2021
Hydrogen & Fuel Cells Day

https://science.osti.gov/bes/Community-Resources/Reports

Roundtable Report:

- Undergoing final edits by Co-Chairs
- "functional draft" to BES by December 10, 2021
- Plan to release report in early CY22

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- ORNL Production Team

Thanks to the entire team!

Thank you for your attention

Questions?

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