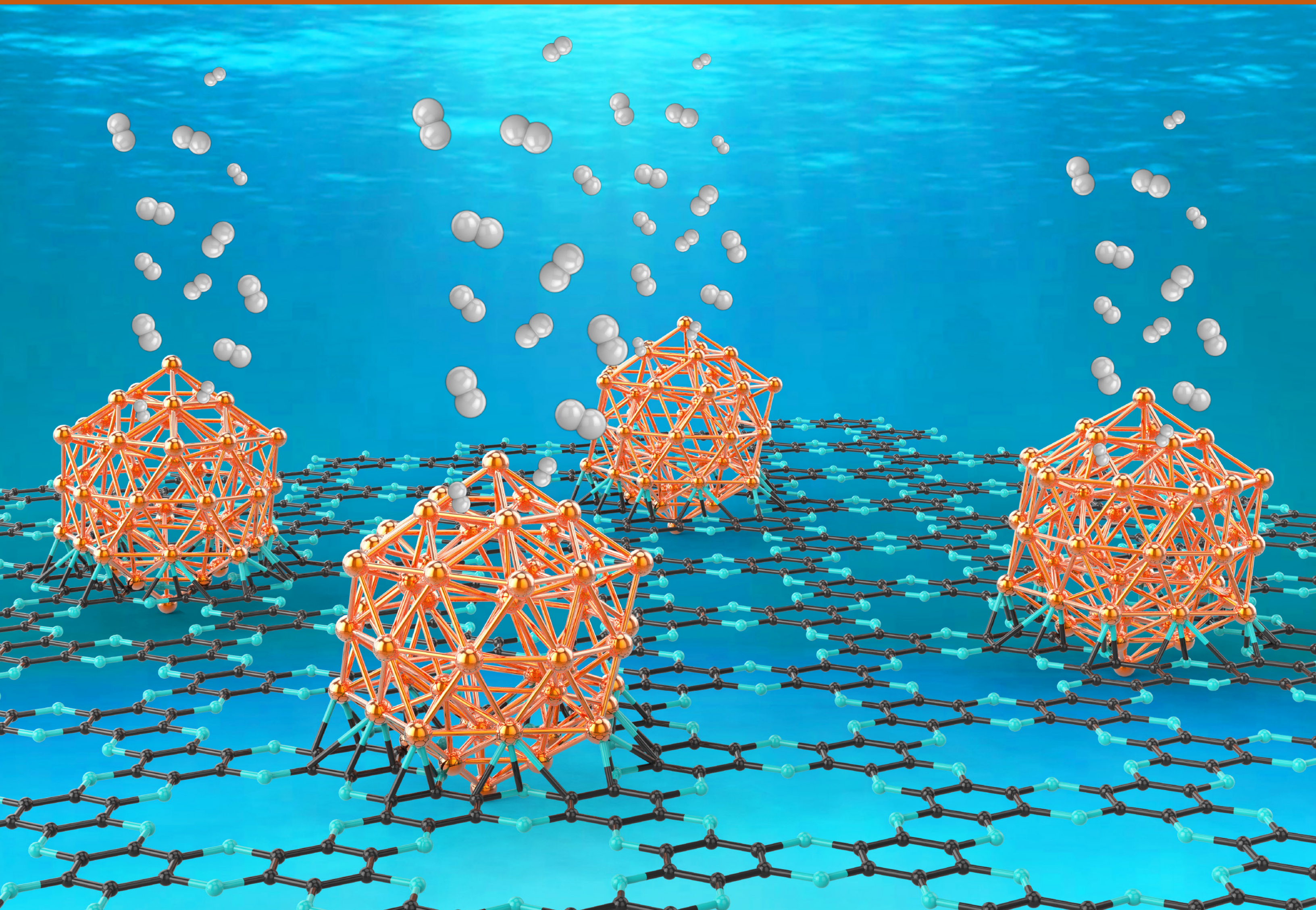
Basic Energy Sciences Roundtable

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

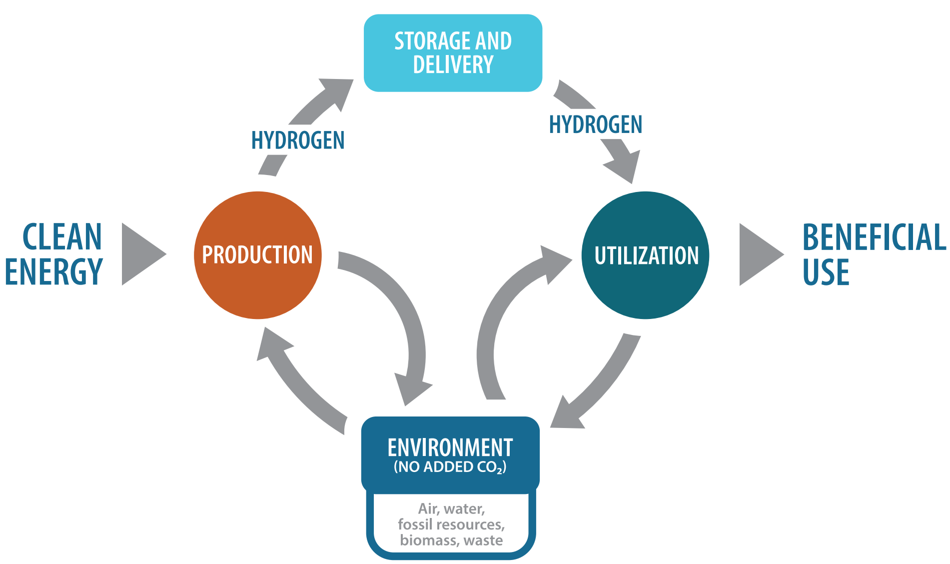
Scientific Breakthroughs are Needed to Enable Carbon-Neutral Hydrogen Technologies

The most abundant element in the universe is hydrogen, a lightweight element that plays a massive role in how energy is stored and used. The simplicity of the bond between the two hydrogen atoms that form a hydrogen molecule belies the complexity of efficient hydrogen use to address today's global energy challenges. The amount of hydrogen used worldwide is enormous; about 70 million metric tons are produced globally every year and used in oil refining, chemical production, especially for ammonia, steel manufacturing, transportation fuels, and more. Hydrogen is an increasingly crucial component for carbon-neutral energy systems both as a clean way to store energy for future use (i.e., as an energy carrier) and as a chemical feedstock. Thus, there is a compelling need for innovations to enable hydrogen technologies that do not emit carbon dioxide (i.e., are carbon neutral).

Hydrogen can be produced by water splitting, by catalytic or thermal cracking of methane, from microorganisms under mild biological conditions, and from biomass through integrated catalytic processes. Hydrogen must be safely transported and stored by using novel materials and chemical storage strategies. Progress has been made in hydrogen research over the previous two decades; however, fundamental research is required to overcome the technical hurdles that continue to limit the implementation of economically viable systems and processes for carbon-neutral hydrogen production, storage, and utilization.

Basic research to identify and understand the fundamental principles governing hydrogen processes is essential for achieving a carbon-neutral, hydrogen-based energy and chemical infrastructure. In August 2021, the Office of Basic Energy Sciences (BES)—in coordination with the US Department of Energy (DOE) technology Offices of Energy Efficiency and Renewable Energy, Fossil Energy and Carbon Management, and Nuclear Energy—held a roundtable titled, "Foundational Science for Carbon-Neutral Hydrogen Technologies," to discuss the scientific and technical barriers for carbon-neutral hydrogen production, storage, and utilization. Four priority research opportunities were identified to address these scientific and technical challenges and accelerate progress toward the realization of energy-efficient, carbon-neutral cycles for hydrogen processes.

A technology status document developed for the roundtable and the full report will be posted at: https://science.osti.gov/bes/Community-Resources/Reports.



The Carbon-Neutral Hydrogen Cycle:

Production: Generation of hydrogen using clean energy sources

Storage and Delivery: Hydrogen storage and delivery using materials or chemical storage methods

Utilization: Use of hydrogen as a clean-energy carrier to power processes or as a chemical feedstock

Priority Research Opportunities

- **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.

- **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.

- **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.

- **Understand and Limit Degradation Processes to Enhance the Durability of Hydrogen Systems**

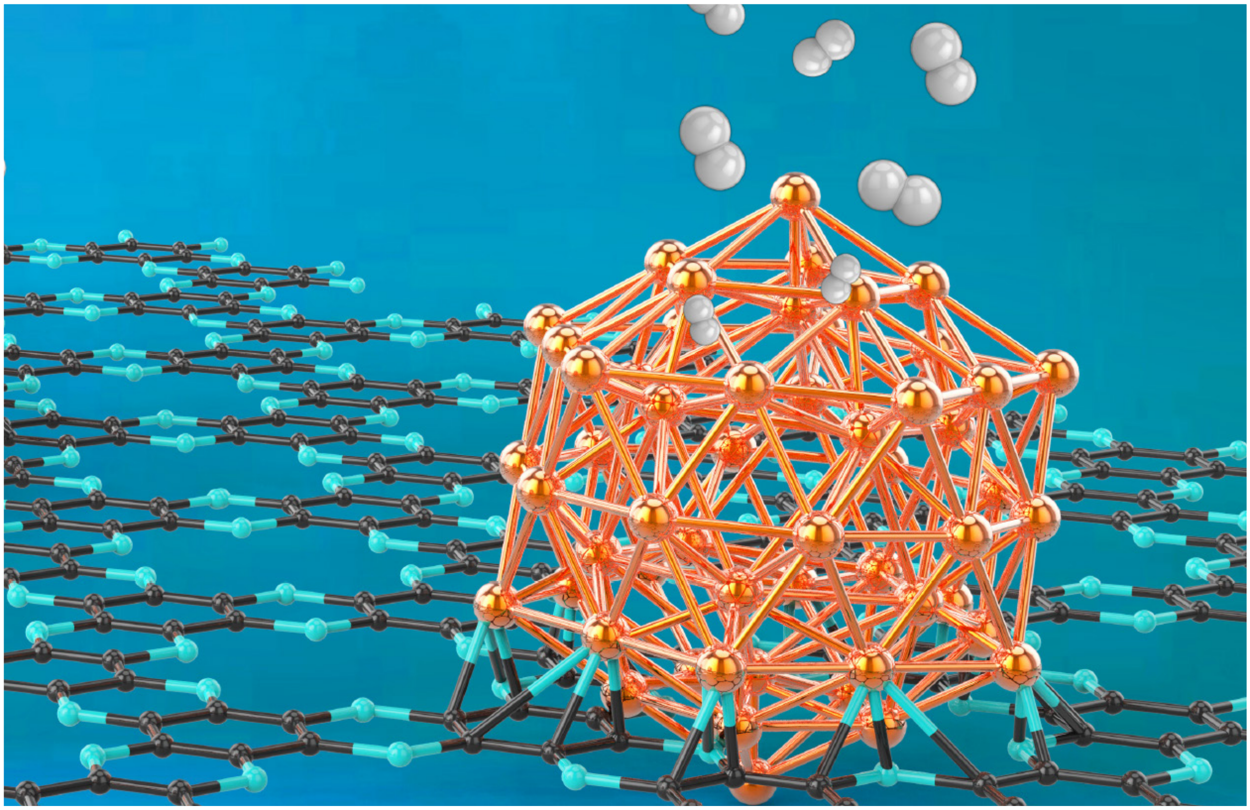
  Key question: *How can we identify and understand the complex mechanisms of degradation to obtain foundational knowledge that enables the predictive design of robust hydrogen systems?*

  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.

Summary

The scientific and technical barriers associated with carbon-neutral hydrogen production, chemical- and materials-based hydrogen storage, and utilization in technologies were identified and integrated into four priority research opportunities. These opportunities provide a cogent framework for greatly accelerating the design and development of materials and processes required for carbon-neutral hydrogen systems. These outcomes build upon and go well beyond research opportunities outlined in previous BES workshops and recent DOE reports; identify the most significant avenues for discovering and developing selective, stable, and efficient chemical and materials systems; and will create a paradigm shift in the foundational science to enable innovative carbon-neutral hydrogen technologies.

Advances will be realized by integrating novel, operando experimental techniques; predictive theory and modeling; and analytical data science methods. Such progress will enable innovative chemical and materials synthesis, further understanding of hydrogen interactions with molecules and materials, tracking the evolution of complex interfaces, and elucidating pathways to mitigate critical degradation processes. Research based on the priorities outlined here will greatly impact hydrogen production, storage, and utilization of systems and processes and will provide the scientific foundation for clean future technologies based on the remarkably versatile chemistry of hydrogen.



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