
Hydrogen Fuel R&D Subprogram Overview

INTRODUCTION

The Hydrogen Fuel R&D subprogram focuses on early-stage research and development (R&D) to reduce the cost and improve the reliability of technologies used to produce and store hydrogen from diverse domestic energy resources. The hydrogen delivery component of the subprogram was transferred into the new Hydrogen Infrastructure R&D line item in the fiscal year (FY) 2019 President's Budget Request and received appropriations under that line item. In support of R&D needs identified through the U.S. Department of Energy's (DOE's) H2@Scale efforts, the Hydrogen Fuel R&D subprogram is developing a portfolio of hydrogen production and storage technology pathways. The subprogram addresses technical challenges through a portfolio of projects in two R&D areas:

- **Hydrogen production** addresses low-cost, highly efficient hydrogen production technologies that utilize diverse domestic sources of energy. Early-stage R&D activities include advanced water splitting and innovative concepts such as biological hydrogen production. The former is predominantly coordinated through the HydroGEN Advanced Water Splitting Materials consortium (HydroGEN) to accelerate research, development, and deployment of advanced water splitting technologies for clean, sustainable hydrogen production.
- **Hydrogen storage** addresses cost-effective onboard and offboard hydrogen storage technologies with improved energy density. Early-stage R&D activities include high-pressure compressed storage, materials-based storage, and hydrogen carriers. The latter two are coordinated through the Hydrogen Materials—Advanced Research Consortium (HyMARC) to accelerate the discovery of breakthrough hydrogen storage materials.

In FY 2018, hydrogen production projects focused primarily on early-stage R&D for advanced water splitting materials and systems funded through HydroGEN, which is part of the DOE Energy Materials Network. Production pathways under investigation included advanced high- and low-temperature electrochemical water splitting (HTE, LTE), direct solar thermochemical (STCH) and photoelectrochemical (PEC) water splitting, and novel reforming processes for hydrocarbon and waste-stream feedstocks (including thermal, catalytic, and microbial-based processes). Hydrogen storage projects in FY 2018 focused on materials-based hydrogen storage R&D through HyMARC and on advanced tanks through development of precursor fibers for low-cost carbon fiber.

GOALS

The Hydrogen Fuel R&D subprogram goals are to develop:

- Low-cost, highly efficient technologies for *hydrogen production* from diverse domestic resources for both centralized and distributed production applications
- Innovative, low-cost, and energy-dense *hydrogen storage* technologies for transportation and stationary applications, including niche areas such as portable power and material handling equipment.

OBJECTIVES

The Hydrogen Fuel R&D subprogram evaluates its project portfolio with respect to its potential to meet DOE's ultimate cost targets of <\$2 per kilogram (or gasoline gallon equivalent, gge) for hydrogen production and \$8/kWh for hydrogen storage systems while achieving 2.2 kWh/kg and 1.7kWh/L for hydrogen storage system gravimetric and volumetric energy densities, respectively. Interim objectives, consistent with DOE's H2@Scale vision, include:

- Reduce the cost of *hydrogen production* from diverse domestic resources to $< \$2/\text{kg}$ (with a near-term target of $< \$7/\text{kg}$ and an ultimate target of $< \$4/\text{kg}$ for delivered and dispensed hydrogen). This cost is independent of the technology pathway and takes into consideration a range of assumptions for fuel cell electric vehicles (FCEVs) to be competitive.
- Develop *hydrogen storage* systems achieving 1.8 kWh/kg and 1.3 kWh/L for gravimetric and volumetric densities, respectively, at a cost of $\$9/\text{kWh}$ by 2025.

FY 2018 TECHNOLOGY STATUS AND ACCOMPLISHMENTS

The Hydrogen Fuel R&D subprogram actively monitors the technical progress achieved through the hydrogen production and storage project portfolios and incorporates that progress into the status of the technology with respect to performance metrics such as cost, efficiency, and energy density.

Figure 1 shows recent and current status for the high-volume projected costs of hydrogen production for several of the near- to mid-term production pathways, highlighting the cost reductions in recent years resulting from ongoing early-stage R&D. Although natural gas reforming (without carbon capture) already meets the DOE cost target of $< \$2/\text{kg}$, continued early-stage R&D is needed to enable the innovations essential for reducing cost in other large-scale hydrogen production technology pathways utilizing diverse and sustainable domestic resources.

Figure 2 shows the current status of high-pressure compressed hydrogen storage systems for various performance metrics against DOE's ultimate targets. In addition to system cost challenges, compressed hydrogen storage systems are unable to meet the ultimate goal for energy density. The density of hydrogen gas poses a theoretical limitation that prevents ambient compressed hydrogen systems from being able to meet the energy density targets. To address this challenge the subprogram portfolio includes less mature cold/cryo-compressed and materials-based hydrogen storage technologies that have the potential to satisfy all onboard hydrogen storage targets, including energy density.

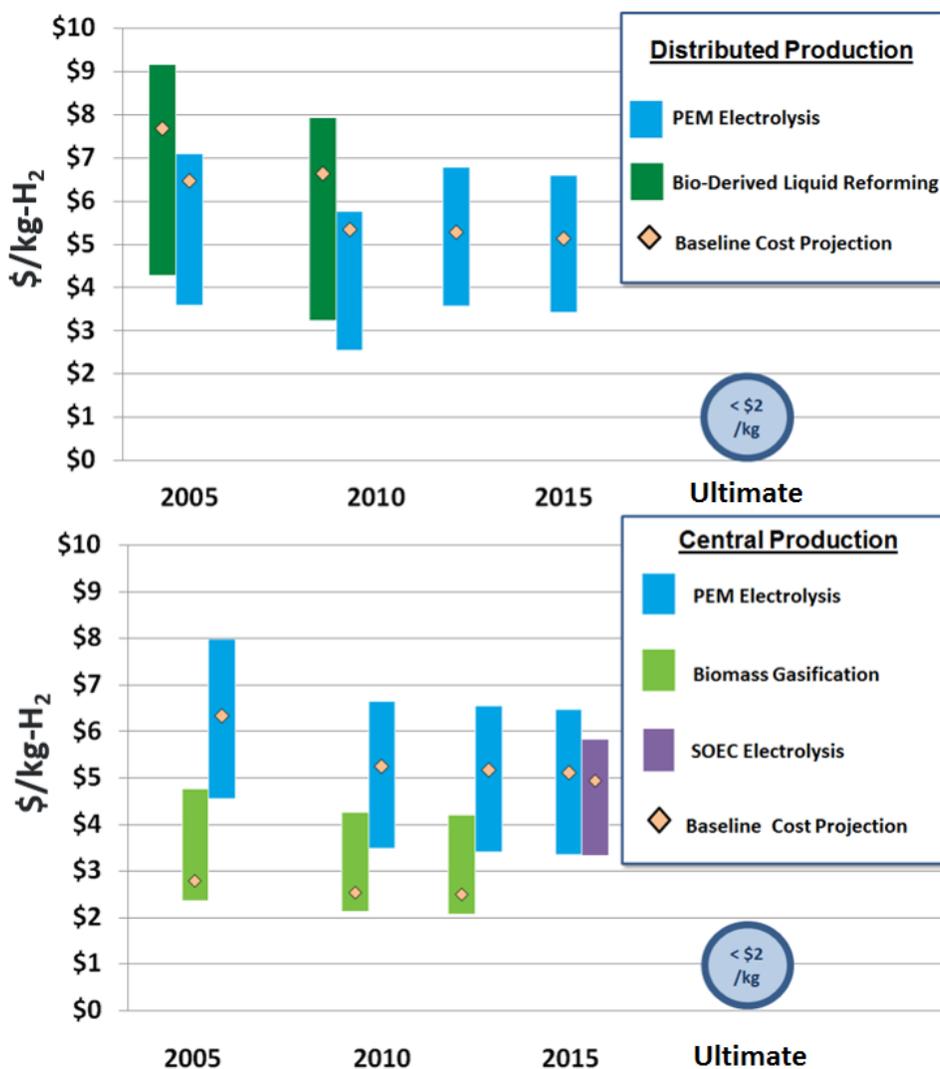


Figure 1. Status for the high-volume projected costs of hydrogen production

Range of hydrogen production costs, untaxed, for near- to mid-term distributed and centralized pathways. The high end of each bar represents a pathway-specific high feedstock cost as well as an escalation of capital cost, while the low end reflects a low feedstock cost and no capital escalation. Bars for different years in the same pathway represent improvements in the costs of the specific pathway, based on specific reference data for the appropriate year and pathway. Detailed information is included in the DOE Hydrogen and Fuel Cells Program Records 14005¹ and 16014.²

¹ *Hydrogen Production Status 2006-2013*, Program Record (Hydrogen and Fuel Cells Program) 14005, U.S. Department of Energy, 2014. https://www.hydrogen.energy.gov/pdfs/14005_hydrogen_production_status_2006-2013.pdf

² *Hydrogen Production Cost from Solid Oxide Electrolysis*, Program Record (Hydrogen and Fuel Cells Program) 16014, U.S. Department of Energy, 2016. https://www.hydrogen.energy.gov/pdfs/16014_h2_production_cost_solid_oxide_electrolysis.pdf

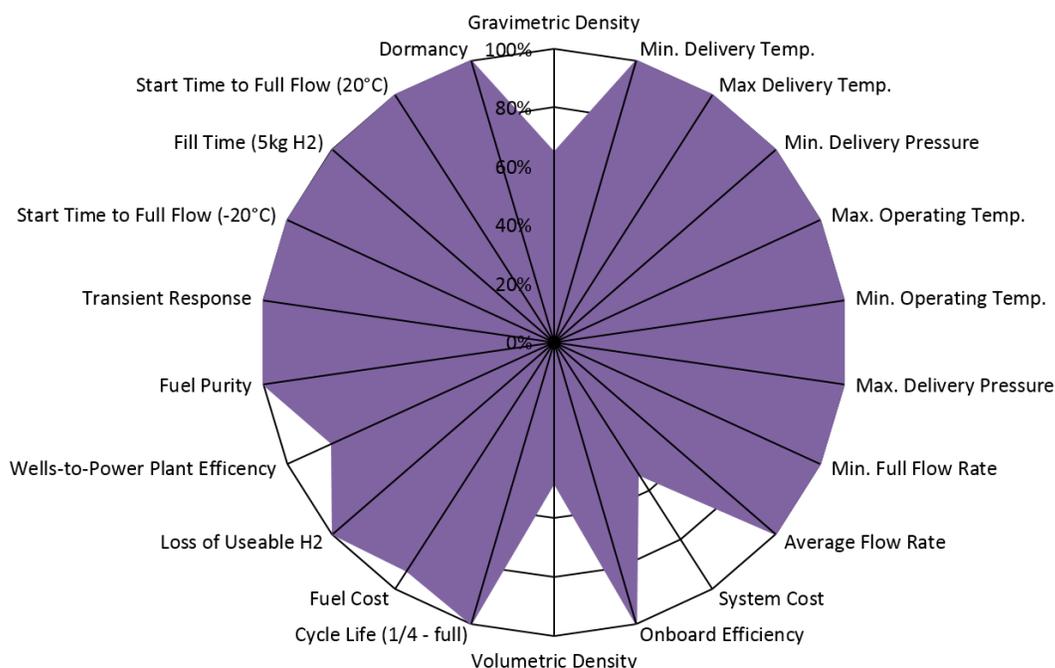


Figure 2. Current status of high-pressure compressed hydrogen storage systems

Current projected performance of a state-of-the-art 700-bar compressed hydrogen storage system with 5.6 kg usable hydrogen storage with ultimate onboard automotive targets³

Subprogram-Level Accomplishments

The Hydrogen Fuel R&D subprogram made significant progress on several fronts during FY 2018. Specific examples include the following.

Hydrogen Production

- The HydroGEN consortium incorporated 19 new funding opportunity announcement (FOA)-awarded projects working across the four advanced water splitting (AWS) technologies and leveraging the capabilities and expertise of six core national laboratories—National Renewable Energy Laboratory (NREL), Sandia National Laboratories (SNL), Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL), Idaho National Laboratory (INL), and Savannah River National Laboratory (SRNL)—to accelerate materials research in order to advance the development of water splitting technologies.
- HydroGEN successfully engaged in an interagency collaboration with the National Science Foundation’s (NSF) Designing Materials to Revolutionize and Engineer our Future (DMREF) program element, resulting in four NSF DMREF projects that will leverage HydroGEN’s expertise and capabilities in three water splitting technologies (PEC, LTE, and STCH).
- The subprogram engaged stakeholders with the release of a Request for Information entitled “H2@Scale: Determining Opportunities to Facilitate Wide-Scale Hydrogen Adoption for Energy Security and

³ *Fuel Cell System Cost—2015*, Program Record (Hydrogen and Fuel Cells Program) 15015, U.S. Department of Energy, 2015. https://www.hydrogen.energy.gov/pdfs/15015_fuel_cell_system_cost_2015.pdf

Economic Growth.” This resulted in more than 70 responses from academic, national laboratory, and industry stakeholders providing their experience and expertise on expanding hydrogen production at large scale across the United States.

- R&D projects in the current hydrogen production portfolio made significant progress, including advances in early-stage materials research for advanced low- and high-temperature electrolysis (including catalyst and membrane innovations); advances in materials research foundational to the PEC and STCH pathways (including novel energy-conversion materials and catalysts); and progress in cutting-edge metabolic engineering for enabling early-stage biological approaches to the conversion of hydrocarbon feedstocks based on biomass and waste streams. The progress is described in further detail in the project-level accomplishments section below.

Hydrogen Storage

- In FY 2018, the hydrogen storage activity negotiated a four-year second phase for the HyMARC effort. For the second phase, the core national laboratory team is being expanded beyond the initial national laboratory team of SNL, LLNL, and LBNL to include NREL, Pacific Northwest National Laboratory (PNNL), the SLAC National Accelerator Laboratory, and the National Institute of Standards and Technology (NIST) Center for Neutron Research, thus fully integrating the former “HySCORE” team into HyMARC. In support of the H2@Scale initiative, second-phase HyMARC activities will include performing foundational research on hydrogen carriers for bulk hydrogen storage and transport as well as on materials for onboard vehicle storage.
- The subprogram completed Phase I go/no-go decisions on seven of the nine initial seedling projects selected through the FOAs in FY 2016 and 2017. Three projects met their go criteria and will be supported for additional research. Four projects did not meet their go criteria and the projects have been discontinued. The two remaining seedling projects are scheduled to complete their Phase I efforts in early FY 2019.
- With support from the subprogram, the HyMARC team published two significant peer-reviewed papers in FY 2018 to provide guidance to researchers developing viable hydrogen storage materials. First was a perspective article titled “An assessment of the strategies for the development of solid-state adsorbents for vehicular hydrogen storage” in the journal *Energy and Environmental Science*. The second was a review paper titled “Nanostructured Metal Hydrides for Hydrogen Storage” in the journal *Chemical Reviews*.
- The subprogram initiated a new effort to evaluate materials for use in cryogenic hydrogen applications, specifically for those applications that require a high number of pressure and temperature cycles, such as cryo-compressed and cryo-sorbents storage. This effort, which will be incorporated into the new Hydrogen Materials (H-Mat) Consortium activities, is being led by PNNL and includes participation from SNL, Oak Ridge National Laboratory (ORNL), and Argonne National Laboratory (ANL).

New Project Selections

In FY 2018, the Hydrogen Fuel R&D subprogram added three HTE projects to support early-stage R&D efforts addressing critical challenges and barriers to hydrogen production via water splitting. The three projects are listed below:

- FuelCell Energy will develop advanced high-temperature water splitting systems for production of hydrogen through efficient and durable electrolytic cells and stacks using innovative proton-conducting ceramic materials and operating at a temperature $\geq 500^{\circ}\text{C}$.
- West Virginia University, through the HydroGEN consortium, will develop new HTE materials capable of durable and efficient operation at temperatures compatible with nuclear energy heat sources. Their

innovations will focus on solving the low performance/high degradation of solid oxide electrolysis cells by developing intermediate-temperature proton-conducting solid oxide electrolysis cells with robust electrode structure and intrinsically advantageous electrode kinetics.

- Saint-Gobain, through the HydroGEN consortium, will develop durable materials for cost-effective advanced water splitting utilizing all-ceramic solid oxide electrolyzer stack technology. They will focus on adapting their novel, all-ceramic stack technology to HTE with a focus on addressing fundamental durability challenges.

Project-Level Accomplishments

During FY 2018, projects in the Hydrogen Fuel R&D portfolio made important progress in several key areas. Examples include the following.

Electrolytic Hydrogen Production

- Achieved cell performance of 1.39 V at 600 mA/cm² for over 30 hours in a high-temperature alkaline electrolyzer using molten hydroxides in porous zirconia matrix as the electrolyte demonstrating a first-of-its-kind high-temperature electrolysis system. (Giner, Inc.)

Biological Conversion of Hydrocarbon Feedstocks for Hydrogen Production

- Demonstrated hydrogen production with a yield of 8.5 mol H₂/mol glucose, just shy of the 2020 target of 9 mol H₂/mol glucose with a novel 10 L hybrid fermentation and microbial electrolysis cell reactor system. (Oregon State University)

HydroGEN Project Accomplishments

The HydroGEN consortium fosters cross-cutting materials innovation using theory-guided applied materials research and development to advance all emerging thermochemical and electrolysis AWS pathways (LTE, HTE, PEC, and STCH), including hybridized systems. Throughout FY 2018 HydroGEN has fostered collaboration between the core national laboratories and industry and academic partners resulting in the exchange of more than 100 material samples, the engagement of 150 collaborators using the web hosting site, 26 published articles, two records of inventions, 44 unique resource nodes utilized by project partners, the establishment of a literature database, and expansion of a data hub for facile sharing and dissemination of data to the scientific community with more than 100 users and nearly 4,000 data files to date. The following highlights are from the HydroGEN seedling projects that are leveraging HydroGEN capabilities to accelerate their materials R&D.

Low-Temperature Electrolysis Materials R&D

- Demonstrated advanced membrane electrode assembly with performance of 1.8 A/cm² at <1.7 V, exceeding near-term performance targets of 1.8 A/cm² at 1.85 V, using next-generation cell components and demonstrated 800 hours of durability at 2 A/cm², operating at 80°C and 30 bar. (Proton Onsite)
- Successfully fabricated novel alkaline exchange membranes via a low-cost synthesis approach based on acid-catalyzed condensation reaction. (LANL)
- Developed two series of metal organic framework-derived platinum group metal (PGM)-free oxygen evolution catalysts for polymer electrolyte membrane electrolyzers, both of which demonstrated less than 15 mV difference (<2% difference) from the state of the art. (ANL)

High-Temperature Electrolysis Materials R&D

- Developed an experimentally validated model for electrolyte degradation in solid oxide electrolysis cells to predict the conditions where electrolyte failure occurs. (Northwestern University)

- Demonstrated a proton-conducting electrochemical cell with a performance of 1.2 A/cm² at <1.4 V and ≤650°C, which meets the target of >1 A/cm² at <1.4 V. (University of Connecticut)
- Developed a metal-supported, proton-conducting electrolyte button cell using a novel process for electrolyte deposition, exceeding performance targets of 0.8 A/cm² at 1.4 V. (United Technologies Research Center)

Photoelectrochemical Materials R&D

- Achieved a solar-to-hydrogen efficiency of 11.5% with a PGM-free Ni₅P₄ hydrogen evolution catalyst integrated with a high-performing photoabsorber, exceeding the target of 10% efficiency and on par with conventional PtRu catalysts. (Rutgers)
- Demonstrated a GaN/Si photocathode with stable operation for >100 hour at high photocurrent density of ~38 mA/cm², without surface protection. (University of Michigan)
- Demonstrated >100-hour stability for a III-V photocathode with a non-precious metal hydrogen evolution catalyst at >10 mA/cm² under 1-sun, meeting the target. (Stanford)

Solar Thermochemical Materials R&D

- Developed machine learning models for the discovery of efficient and stable STCH materials, identifying ~28,000 stable perovskite formulations from more than 1.1 million possible candidates with more than 90% accuracy. (University of Colorado Boulder)
- Demonstrated >200 μmol H₂/g with three compositions of Ce_xSr_{2-x}MnO₄, significantly exceeding the target of 59 μmol H₂/g (based on the performance of ceria under similar conditions). (Colorado School of Mines)

High-Pressure Compressed Hydrogen Storage

- Demonstrated lower-cost polyacrylonitrile (PAN) feedstock material fiber spinning and conversion to high strength carbon fiber, resulting in 14% cost reduction compared to the current PAN. Also demonstrated efficient solvent recovery and reduced fresh water use. (University of Kentucky)
- Developed four new low-cost polyolefin- and polyethylene-pitch-based precursors with >80% carbon yield. (Penn State University)
- Demonstrated >10°C decrease in PAN melt temperature using ionic liquid as plasticizer. The decreased PAN melt temperature enables the melt spinning process, which indicates a potential 50% cost reduction in the production process compared to conventional wet spinning. (Oak Ridge National Laboratory)

Advanced Materials-Based Hydrogen Storage

The HyMARC lab team completed activities that established an improved understanding about scientific gaps impeding the advancement of solid-state storage materials. Some of these include:

- Determined and validated an accurate Mg-B-H phase diagram that includes high-pressure and high-temperature regimes. (LLNL/SNL/PNNL)
- Accurately determined the enthalpy and entropy of hydrogen desorption in bulk Mg(BH₄)₂, addressing a gap in the literature. (SNL)

- Computationally determined that introduction of boron into coronene, as a model system for activated carbon, provides no improvement in binding energy for several optimized, stable structures. (PNNL/NREL)
- Assessed potential of confinement stress/strain to tune thermodynamics and kinetics of hydrogen uptake and release. (LLNL/LBNL)
- Elucidated the sorption mechanisms for complex hydrides and established that titanium doesn't play a role on the material surface; however, oxides do for NaAlH₄ desorption. (SNL/LBNL/LLNL)

HyMARC Project Accomplishments

The HyMARC seedling projects are high-risk, high-reward projects that focus on material development and rely heavily on the HyMARC core national lab team for guidance to accelerate their materials development efforts through computational, synthetic, characterization, and validation capabilities. Examples of progress achieved by the HyMARC seedling projects include:

- Demonstrated hydrogenation of MgB₂ to Mg(BH₄)₂ at 25% lower temperature and 22% lower pressure than prior state of the art. (University of Hawaii)
- Demonstrated that the addition of an electrolyte facilitates a 10x improvement in dehydrogenation kinetics for Mg(BH₄)₂ compared to the bulk material. (Liox Power)
- Demonstrated the ability to form Al₂O₃ coating on Mg(BH₄)₂ nanoparticles with improved reversibility and kinetics. (NREL)
- Identified more than 69,000 real and hypothetical metal organic framework structures with the potential to outperform the current state-of-the-art material through computational machine learning techniques. (University of Michigan)

Technoeconomic Analysis

The subprogram also continued carrying out technoeconomic assessments of hydrogen production and storage technologies to ensure the overall portfolio is heading toward meeting DOE's ultimate goals. Examples of analysis activities in FY 2018 include:

- Completed the update of the H2A (Hydrogen Analysis) Production model to v3.2018. The new version has been released and is available at https://www.hydrogen.energy.gov/h2a_production.html. It includes updates to feedstock costs (Annual Energy Outlook 2017), reference dollar years (2016\$), and plant start dates for current (2015) and future (2040) scenarios. H2A v3.2108 also includes changes to the financing default from 100% percent equity to 40% equity, and the federal tax rate from 35% to 21%. A significant change is the ability to analyze cases using constant debt-to-equity ratio over the plant life, which is a new H2A default. Previously published case studies have been updated to the new version of the model.
- Performed initial analysis of three potential hydrogen carriers for bulk hydrogen transport and compared the cost and energy efficiency of compressed hydrogen delivery. This initial analysis focused on delivery to a terminal at a city gate with a hydrogen demand of 50,000 kg per day. The capital costs for the carrier production and dehydrogenation facilities were identified as key costs that need to be lowered to improve carrier competitiveness. (ANL)

BUDGET

The FY 2018 appropriation for the Hydrogen Fuel R&D subprogram totaled \$38 million. The hydrogen production and storage R&D portfolios were funded at \$22 million and \$16 million, respectively. The hydrogen delivery portion is described in the Technology Acceleration and Hydrogen Infrastructure R&D section of the Annual Progress Report. The estimated budget breakdown for the hydrogen production and hydrogen storage portfolio is shown in Figure 3 and Figure 4.

Funds going toward the hydrogen storage portfolio supported a variety of early-phase R&D efforts on advanced hydrogen storage materials, including hydrogen carriers, and allowed for their coordination through HyMARC to ensure impact was maximized and resources were effectively utilized. Hydrogen storage funding also supported innovative R&D to lower the cost of high-pressure storage systems through low-cost carbon fiber precursor processing and alternative fibers.

Funds going toward hydrogen production supported R&D projects advancing direct solar water splitting, advanced electrolysis, innovative concepts, and benchmarking and analysis.

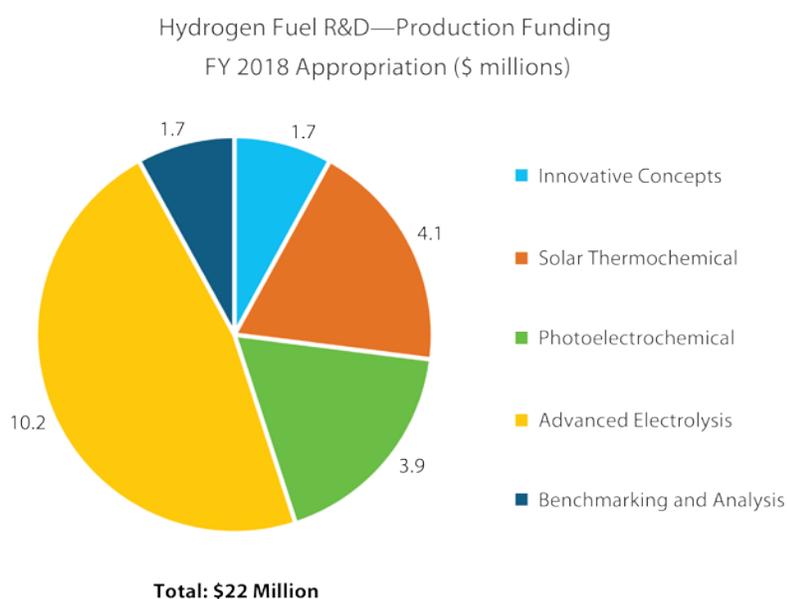


Figure 3. Hydrogen Fuel R&D subprogram FY 2018 appropriation for hydrogen production activities

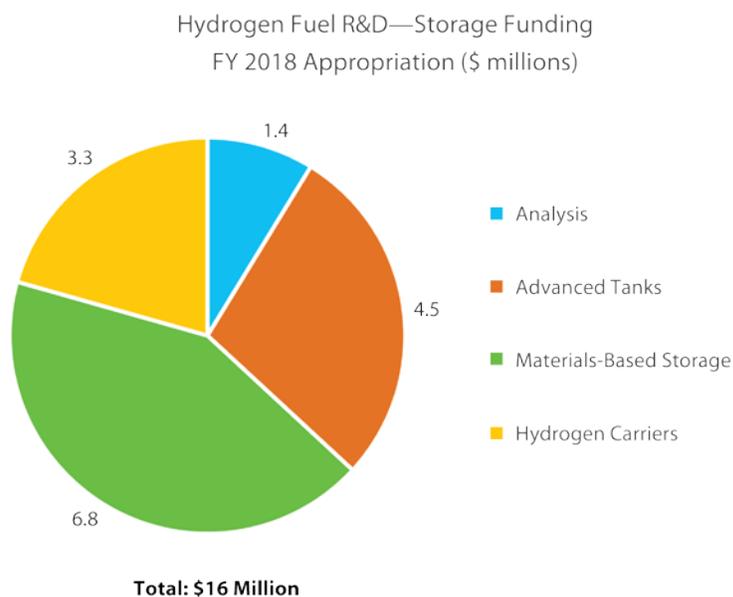


Figure 4. Hydrogen Fuel R&D subprogram FY 2018 appropriation for hydrogen storage activities

UPCOMING ACTIVITIES AND PLANS

The Hydrogen Fuel R&D subprogram will continue efforts to maximize early-stage R&D in advanced hydrogen production and storage technologies with the potential to meet DOE's ultimate targets. In addition, the subprogram will initiate the following activities in FY 2019:

- Pursue early-stage R&D in the bulk storage and transportation of hydrogen, including hydrogen carriers, to support the H2@Scale initiative
- Expand early-stage R&D in materials-based storage to identify promising materials with the potential to store hydrogen and natural gas onboard heavy-duty transportation applications
- Continue support of foundational research needs in hydrogen production identified through H2@Scale efforts, including continued emphasis on research innovations for enhancing efficiency and durability and reducing costs in materials systems for all hydrogen production pathways
- Expand early-stage R&D through the HydroGEN Advanced Water Splitting Materials consortium, including Phase II of the 19 projects and ongoing enhancement of the HydroGEN national laboratory core capabilities in advanced electrochemical, PEC, and thermochemical water splitting
- Expand emphasis on the development of robust materials-characterization protocols and performance-benchmarking standards to verify the potential of materials innovations
- Continue leveraging cross-office and cross-agency R&D opportunities and resources, including expanded collaboration with the NSF, the DOE Office of Basic Energy Sciences program in solar fuels, and the Advanced Research Projects Agency-Energy.
- Launch the BioH2 consortium aimed at addressing several technical barriers that must be overcome to realize technoeconomic feasibility of biological hydrogen production to meet the DOE hydrogen

production cost goal of <\$2/kg. By leveraging the world-class capabilities and scientific expertise of the national laboratories, the multi-lab BioH2 consortium will deliver the multidisciplinary and synergistic expertise to address technical barriers associated with fermentation and microbial electrolysis cells.

Eric Miller

Hydrogen Production Subprogram Manager
Fuel Cell Technologies Office
Office of Energy Efficiency and Renewable
Energy
U.S. Department of Energy
1000 Independence Ave., SW
Washington, DC 20585-0121
Phone: (202) 586-5829
Email: Eric.Miller@ee.doe.gov

Ned Stetson

Hydrogen Storage Subprogram Manager
Fuel Cell Technologies Office
Office of Energy Efficiency and Renewable
Energy
U.S. Department of Energy
1000 Independence Ave., SW
Washington, DC 20585-0121
Phone: (202) 586-9995
Email: Ned.Stetson@ee.doe.gov