II.0 Hydrogen Production Sub-Program Overview

INTRODUCTION

The Hydrogen Production sub-program supports early-stage research and development (R&D) of technologies that will enable the long-term viability of hydrogen as an energy carrier for a diverse range of end-use applications including transportation (e.g., specialty vehicles, cars, trucks, and buses), stationary power (e.g., backup power and combined heat and power systems), portable power (e.g., auxiliary power units), and chemical processing (e.g., fertilizer production, oil refining, and methanol production). In support of R&D needs identified through the U.S. Department of Energy's (DOE's) H2@Scale efforts, the Hydrogen Production sub-program is developing a portfolio of hydrogen production technology pathways utilizing a variety of sustainable domestic energy sources and feedstocks.

The Fuel Cell Technologies Office, within DOE's Office of Energy Efficiency and Renewable Energy, is developing technologies that include advanced electrochemical water splitting (including high temperature/pressure operations and novel catalysts/membranes), direct solar water splitting (including thermochemical and photoelectrochemical processes), as well as novel reforming processes of hydrocarbon and waste-stream feedstocks (including thermal, catalytic, and microbial-based processes).

Complementing the Fuel Cell Technologies Office efforts, multiple DOE offices are engaged in synergistic R&D that is relevant to hydrogen production, including:

- The Office of Science's Basic Energy Sciences program conducts research to expand the foundational understanding of processes and mechanisms relevant to hydrogen production, including interfacial phenomena, light-matter interactions, and fundamental thermodynamics and kinetics; such mechanisms are specifically relevant to photoelectrochemical and thermochemical water splitting, catalysis and electrocatalysis, membranes for gas separation, and biological and biomimetic processes.
- The Office of Nuclear Energy is currently collaborating with the Office of Energy Efficiency and Renewable Energy on the development of nuclear-renewable hybrid energy systems that are consistent with the H2@Scale vision. The systems being evaluated in this collaboration use large-scale hydrogen production as a form of energy storage or as an input to industrial processes.
- The Office of Fossil Energy is advancing the technologies for producing hydrogen from fossil fuel resources, including co-production of hydrogen and electricity and steam methane reformation. The Office of Fossil Energy also continues to develop technologies for carbon capture, utilization, and storage in fossil-based hydrogen production, including technologies for carbon-free production of hydrogen using new chemical synthesis methods that break apart natural gas to solid carbon and hydrogen.

GOAL

The goal of the Hydrogen Production sub-program is to implement early-stage applied R&D for developing low-cost, highly efficient hydrogen production technologies that utilize diverse domestic sources of energy, including sustainable and renewable resources (Office of Energy Efficiency and Renewable Energy), nuclear power (Office of Nuclear Energy), and fossil resources with carbon sequestration and utilization (Office of Fossil Energy).

OBJECTIVES

The objective of the Hydrogen Production sub-program is the development of low-cost, large-scale hydrogen production technologies that utilize diverse, domestic energy resources and feedstocks. This objective is consistent with DOE's H2@Scale vision. Analysis has established a long-term hydrogen cost target of <$4 per kilogram (kg) hydrogen, produced, delivered, and dispensed, but untaxed[1] (with <$2/kg apportioned for production only[2]); and a nearer-term, early-market target of <$7/kg dispensed hydrogen[3]. These cost targets are based on achieving cost

[1] *Hydrogen Threshold Cost Calculation*, Program Record (Office of Fuel Cell Technologies) 11007, U.S. Department of Energy, 2011. http://www.hydrogen.energy.gov/pdfs/11007_h2_threshold_costs.pdf

[2] *H_2 Production and Delivery Cost Apportionment*, Program Record (Hydrogen and Fuel Cells Program) 12001, U.S. Department of Energy, 2012. http://hydrogen.energy.gov/pdfs/12001_h2_pd_cost_apportionment.pdf

[3] *Early Market Hydrogen Cost Target Calculation—2015 Update*, Program Record (Fuel Cell Technologies Office) 15012, U.S. Department of Energy, 2015. https://www.hydrogen.energy.gov/pdfs/15012_hydrogen_early_market_cost_target_2015_update.pdf

competitiveness on a cents-per-mile basis in hydrogen fuel cell electric vehicles compared with other competing advanced vehicle technologies. Hydrogen production technologies are being developed to achieve cost goals in timeframes appropriate to their current stages of development.

FISCAL YEAR (FY) 2017 TECHNOLOGY STATUS AND ACCOMPLISHMENTS

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/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.

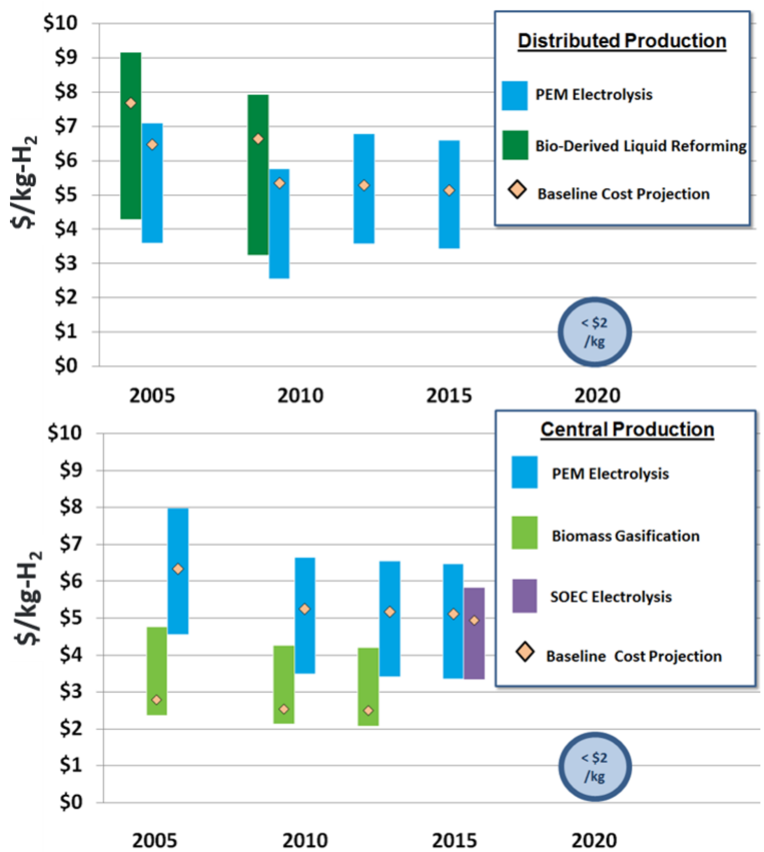

FIGURE 1. Range of hydrogen production costs, untaxed, for near- to mid-term distributed and centralized pathways. The high end of each bar represents a pathway-specific high feedstock cost as well as an escalation of capital cost, while the low end reflects a low end on feedstock costs and no capital 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 14005[4] and 16014[5].

Sub-Program Level Accomplishments

In FY 2017, significant progress was made by the Hydrogen Production sub-program on several important fronts. Several highlights include:

- In FY 2017, DOE announced SimpleFuel as the winner of the $1 million H2 Refuel H-Prize Competition. Launched in October 2014, the H2 Refuel H-Prize Competition challenged America's innovators to deploy

[4] *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

[5] *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

an on-site hydrogen generation system, using electricity or natural gas, to fuel hydrogen vehicles, that can be used in homes, community centers, small businesses, or similar locations. During the competition, SimpleFuel demonstrated that its home-scale refueling appliance can provide a one-kilogram fill to vehicles in 15 minutes or less at 700 bar using hydrogen produced via electrolysis, with a cost-effective design that minimizes setback distances and reduces the physical footprint of the system. SimpleFuel is a collaboration of three companies: Ivys Energy Solutions, McPhy Energy N.A., and PDC Machines.

- The HydroGEN advanced water splitting materials consortium, comprised of six core national laboratories (National Renewable Energy Laboratory, Sandia National Laboratories, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, Idaho National Laboratory, and Savannah River National Laboratory), launched its expanded website featuring an advanced search engine to facilitate access to the consortium's more than 80 unique world-class research capabilities. HydroGEN also launched its data portal in compliance with DOE Energy Materials Network guidelines and requirements.
- Several important stakeholder engagement events were held, including webinars and workshops. Webinar topics included grid-integration of electrolysis as well as detailed descriptions of the Fuel Cell Technologies Office's Energy Materials Network Consortia, including the HydroGEN Consortium. A workshop co-sponsored by the Fuel Cell Technologies Office and the Advanced Manufacturing Office in the Office of Energy Efficiency and Renewable Energy was held on advanced power electronics for electrolyzer and fuel cell applications, and several workshops were held on H2@Scale.
- R&D projects in the current Hydrogen Production sub-program portfolio made significant progress, which included advances in early-stage hydrogen production pathways analysis; progress in early-stage materials research for advanced low- and high-temperature electrolysis (including catalyst and membrane innovations); advances in materials research foundational to the photoelectrochemical (PEC) and solar-thermochemical (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.
- Nineteen new projects were competitively selected in areas of advanced water splitting materials R&D, which leverage the HydroGEN Consortium's core capabilities. Further details are included in the following sections.

New Project Selections

In FY 2017, DOE released one funding opportunity announcement (FOA) to support R&D efforts to address critical challenges and barriers to hydrogen production via water splitting. Specifically, the FOA aimed to leverage the national laboratories' unique capabilities brought together under the HydroGEN Energy Materials Network Consortium to accelerate materials discovery and development. Advanced water splitting pathways of interest include low- and high-temperature electrolysis and PEC and STCH hydrogen production. In addition to the materials R&D topic, the FOA solicited applications for critical protocol and benchmarking development needed across all the advanced water splitting pathways to guide the materials R&D efforts resulting from the FOA, as well as the entire advanced water splitting community.

Eighteen advanced water splitting materials development projects and one benchmarking and protocol development project were selected in FY 2017 under the Production portfolio and will begin work in early FY 2018. The 19 projects are listed below:

Low-Temperature Electrolysis Materials R&D

- Proton Energy Systems, Inc. (Wallingford, Connecticut) will explore an advanced PEM electrolysis membrane electrode assembly composed of cutting-edge membrane and electrode components with optimized materials structures and interfaces, enabling cost reductions in PEM electrolyzers needed to meet long-term DOE targets.
- Los Alamos National Laboratory (Los Alamos, New Mexico) will develop a platinum-group-metal-free catalyst system for an anion exchange membrane electrolyzer allowing for efficient cell performance while substantially lowering cost.
- Northeastern University (Boston, Massachusetts) will perform a comprehensive fundamental exploration of advanced catalysts, electrodes, membranes, and membrane electrode assemblies integrating these components,

for the next generation of anion exchange membrane electrolyzers optimizing catalytic activity, conductivity, and performance.

- Argonne National Laboratory (Lemont, Illinois) will develop high-efficiency, durable platinum-group-metal-free oxygen evolution reaction catalysts for advanced PEM electrolyzers that are expected to be an order of magnitude less costly compared with current state-of-the-art catalysts.
- Los Alamos National Laboratory (Los Alamos, New Mexico) will explore advanced high-performing, durable, and economically viable elastomeric anion exchange membranes for alkaline water electrolysis under high pH conditions with lower gas permeability, greater mechanical stability, and substantially decreased production cost as compared to the state of the art.

High Temperature Electrolysis Materials R&D

- University of Connecticut (Mansfield, Connecticut) will develop novel solid oxide electrolysis cell (SOEC) technology based on proton-conducting electrolytes to enable cost-effective hydrogen production at intermediate temperatures with important operational advantages over the state of the art, resulting in reduced operational costs.
- Northwestern University (Evanston, Illinois) will utilize accelerated materials testing strategies that combine electrochemical life testing with quantitative microstructural and chemical evaluation to produce a predictive theory addressing critical degradation of SOECs and resulting in accelerated testing protocols critical for SOEC technologies.
- United Technologies Research Center (East Hartford, Connecticut) will develop a thin-film, high-efficiency, durable metal-supported SOEC based upon proton-conducting electrolyte operating at intermediate temperatures, offering an innovative electrolysis cell with the potential to meet long-term DOE targets.

Photoelectrochemical Materials R&D

- Rutgers University (New Brunswick, New Jersey) will explore the development of next-generation PEC photoelectrodes based on novel platinum-group-metal-free catalysts and new multi-junction photoabsorber materials to significantly improve durability, efficiency, and cost compared to the current state of the art.
- Stanford University (Stanford, California) aims to develop protective catalyst systems on III-V and silicon-based semiconductors for efficient and durable PEC water splitting devices made from affordable and scalable materials with the potential to meet the DOE long-term goals.
- The University of Hawaii (Honolulu, Hawaii) will utilize their advanced materials modeling/synthesis/characterization approach to design and optimize the next generation of chalcopyrite-based tandem structures as photoelectrodes for PEC water splitting with innovative surface catalysis and protection layers for enhancing device durability towards meeting long-term DOE targets.
- The University of Michigan (Ann Arbor, Michigan) will explore several novel wide-bandgap materials to develop monolithically integrated thin-film, silicon tandem photoelectrodes to enable high-efficiency and stable PEC water splitting devices.
- Los Alamos National Laboratory (Los Alamos, New Mexico) will design and develop an efficient and stable device structure for sustained PEC water splitting leveraging recent materials innovations in perovskite-based photo-absorbers and in oxygen evolution reaction and hydrogen evolution reaction catalysts.

Solar Thermochemical Materials R&D

- Colorado School of Mines (Golden, Colorado) will merge state-of-the-art combinatorial synthesis methods with combinatorial theoretical calculations to accelerate the discovery of new potential materials for use in two-step metal oxide cycles for cost-effective STCH water splitting, establishing a better understanding of fundamental links between oxide structure, chemical composition, and STCH performance and allowing for characterization of new STCH materials that can meet the long-term DOE hydrogen production targets.
- University of Colorado (Boulder, Colorado) will use a computationally accelerated and experimentally validated materials-by-design approach using advanced machine-learned models to optimize material thermodynamic and kinetic properties for solar thermochemical water splitting that meets or exceeds the long-term DOE targets for hydrogen production in terms of efficiency and cost.

- Northwestern University (Evanston, Illinois) will use a joint computational-experimental method, combined with materials design strategies and high-throughput approaches, to rapidly discover and synthesize novel thermochemical materials with properties that significantly exceed the state of the art, focusing first on novel perovskites, as well as exploring the potential of non-stoichiometric, phase-change materials for optimal thermodynamic and kinetic properties.
- Arizona State University (Tempe, Arizona) will accelerate materials discovery for improved STCH materials by developing a fundamental understanding of key thermodynamic properties of redox active, mixed ionic electronic conducting metal oxides, which can stably exist over a range of oxygen stoichiometries, utilizing intelligent, fundamental quantum mechanics investigations.
- Greenway Energy, LLC (Aiken, South Carolina) will explore the development and testing of a new catalytic material to decompose sulfuric acid, a key step of the hybrid sulfur (HyS) STCH cycle. Using a novel catalyst preparation, the project will develop lower-cost catalytic materials, with 30% higher activity and 60% lower activity degradation expected as compared to the state of the art.

Advanced Water Splitting Materials Protocol and Benchmarking Development

- Proton Energy Systems, Inc. (Wallingford, Connecticut) will establish critically needed best practices for screening, characterization, and benchmarking of the advanced water splitting materials and technologies for hydrogen production. The advanced water splitting materials technologies include advanced high-temperature electrolysis, advanced low-temperature electrolysis, and photoelectrochemical and solar thermochemical water splitting.

Project Level Accomplishments

During FY 2017, current projects in the Hydrogen Production research portfolio made important progress in several key areas, including:

Hydrogen Production Pathway Analysis

Three case studies on hydrogen production costs using the H2A v3 tool were completed: (1) the monolithic piston-type bio-oil reformation reactor, (2) the reformer-electrolyzer-purifier (REP) system, and (3) fermentation systems. In these case studies, industrial-scale systems were modeled based on input from key researchers involved in the projects developing these technologies. After the relevant, detailed information from researchers was collected, data was synthesized and amalgamated into base cases with sensitivity analyses. The baseline parameters and sensitivity limits established in each case study were vetted and peer-reviewed by appropriate industry, academic, and national laboratory stakeholders. Results from the Fermentation H2A case study were incorporated into a published, peer-reviewed Hydrogen and Fuel Cells Program Record.[6] (Strategic Analysis, Inc., National Renewable Energy Laboratory, and Argonne National Laboratory)

Electrolytic Hydrogen Production

The major emphases of the low- and high-temperature electrolysis projects were materials innovations to reduce costs and enhance efficiency and long-term durability. Technical progress included:

- Proton Onsite (Wallingford, Connecticut) demonstrated the first successful full non-platinum-group-metal low-temperature electrolyzer stack incorporating alkaline exchange membrane cells, operating for over 500 h with initial performance at <2 V/cell and 500 mA/cm^2.
- Giner Inc. (Newton, Massachusetts) successfully developed innovative approaches for scaling up low-loading (0.2–0.4 mg/cm^2) $Ir/W_xTi_{1-x}O_2$ PEM electrolyzer anode catalysts, which overcome past durability issues. These new scaled catalysts, along with low-loading 3M nanostructured thin-film anodes and baseline Ir black anodes, are being assembled into a final 36-cell, 65 kW stack for long-term durability testing.
- Ceramatec, Inc., (Salt Lake City, Utah) demonstrated cell stability of ~1% current density degradation per 1,000 h at 1.2 V in a button cell for use in a novel high-temperature water splitting technology. The project incorporated macro-features to provide mechanical support of a thin electrolyte and micro-features of the electrodes to decrease electrode losses.

[6] *Hydrogen Production Cost from Fermentation*, Program Record (Hydrogen and Fuel Cells Program) 16016, U.S. Department of Energy, 2017. https://www.hydrogen.energy.gov/pdfs/16016_h2_production_cost_fermentation.pdf

- FuelCell Energy (Danbury, Connecticut) demonstrated a 20-cell SOEC stack using novel high-power-density solid oxide electrolysis cells in an upgraded stack design for use in high-efficiency high-temperature water splitting. At a current density of 2 A/cm^2, the cell voltage was <1.4 V and the overall degradation rate was <0.60% per 1,000 h over >1,000 h of operation.

Photoelectrochemical Hydrogen Production

The main focus of projects in this area was on using state-of-the-art theory, synthesis, characterization, and benchmarking tools to develop innovative PEC materials with improved efficiency and durability. Technical progress included:

- National Renewable Energy Laboratory (Golden, Colorado) established and peer-reviewed a publication of robust protocols for accurately benchmarking PEC solar-to-hydrogen efficiency, which leverage methodologies used to certify the efficiency of multijunction solid-state solar photovoltaic cells. National Renewable Energy Laboratory applied these protocols to validate the world-record solar-to-hydrogen efficiency of 16.2% in novel III-V semiconductor-based photoelectrodes incorporating an inverted metamorphic multijunction architecture.
- University of Hawaii (Honolulu, Hawaii) demonstrated 350-hour durability in novel chalcopyrite PEC photoelectrodes based on efficient copper-gallium-selenium thin films with MoS_2/TiO_2 surface protective layers and implemented advanced electrochemical and spectroscopic characterizations of these photoelectrodes to better elucidate fundamental degradation mechanisms toward the development of improved mitigation strategies for the further durability enhancements needed in thin-film PEC approaches.
- University of California, Irvine (Irvine, California) completed the first in silico demonstration of a stacked-bed particle-based PEC reactor, sustaining indefinite operation at ~4% solar-to-hydrogen efficiency under diurnal excitation conditions using photocatalyst particles with bandgaps based on state-of-the-art materials (Rh-modified $SrTiO_3$ and $BiVO_4$); concentrations of the IO3–/I– redox shuttle within its solubility range; and membrane permeability ensuring that gas crossover poses no safety issues.

Solar Thermochemical Hydrogen Production

Efforts in these projects were directed toward performance enhancement of water splitting by novel, non-volatile metal-oxide-based reaction materials and validating materials innovations in reactor test-beds designed to optimize efficiency of the reaction cycles. Technical progress included:

- Sandia National Laboratories (Livermore, California) had the first successful demonstration of metal-oxide-based STCH hydrogen production in a cascading pressure reactor/receiver prototype system, at a demonstration scale of ~3.5 kW_{th} with a peak rate of 0.2 SLPM H_2 based on CeO_2 material; this demonstration validates a unique testing procedure that is also critical to evaluation of new complex-perovskite-based redox materials for next-generation STCH systems.
- University of Colorado Boulder (Boulder, Colorado) completed successful long-term testing of spray-dried cobalt-doped hercynite redox material for STCH hydrogen production for over 200 cycles in a stagnation flow reactor system; the active particles produced ~300 µmol/g/cycle with no loss in activity between the 100th and 200th cycles, exceeding the project's targeted performance for hercynite and supporting the viability of this material class for use in next-generation STCH systems.

Biological Conversion of Hydrocarbon Feedstocks for Hydrogen Production

The projects in this area focused on novel biological methods such as fermentation and microbial electrolysis to produce hydrogen from biomass-based hydrocarbon resources, using molecular biology and genetic engineering techniques to enhance the hydrogen production potential. Technical progress included:

- National Renewable Energy Laboratory (Golden, Colorado) successfully generated *C. thermocellum* mutants that exhibited ~30% increase in total hydrogen production with a 55% increase in specific rate of hydrogen production compared with un-mutated strains in the fermentation of biomass feedstocks; this accomplishment validates the importance of state-of-the-art metabolic engineering techniques in the ongoing development of viable fermentative approaches for hydrogen production.
- Virginia Polytechnic Institute and State University (Blacksburg, Virginia) enhanced volumetric productivity of in vitro enzymatic hydrogen production from starch, achieving a peak rate of 550 mmol H_2/L/h (compared to the previously reported 320 mmol H_2/L/h), highlighting the potential viability of this early-stage approach.

- Oregon State University (Corvallis, Oregon) demonstrated hydrogen production rates of >10 L/L/day at 40 g/L, 8 h hydraulic retention time, and 15% biomass content by immobilized fermentative cultures; this result is an important step toward enabling innovative hybrid approaches that can integrate fermentation with microbial electrolysis.

BUDGET

The FY 2017 appropriation for Hydrogen Production and Delivery projects totaled $25.4 million. With the emphasis on supporting H2@Scale and on establishing the HydroGEN Advanced Water Splitting Materials Consortium efforts, the apportionment of this funding in the Hydrogen Production portfolio was approximately $16.1 million. This funding supported (1) resource capabilities in the HydroGEN core national laboratories plus the 19 new HydroGEN projects selected in the FY 2017 funding opportunity announcement (~$9.0 million); (2) key H2@Scale initiatives, including $3 million in Congressionally-directed support for R&D in innovative technologies to split natural gas into hydrogen and value-added solid carbon byproducts; (3) ongoing legacy projects in biological approaches to converting hydrocarbons in biomass feedstocks and waste streams (~$0.9 million) and advanced electrochemical and solar water splitting technologies (~$0.97 million); and (4) ongoing analysis, technical support, and cross-cutting projects. The estimated budget breakdown for Hydrogen Production funding in FY 2017 is shown in Figure 2.

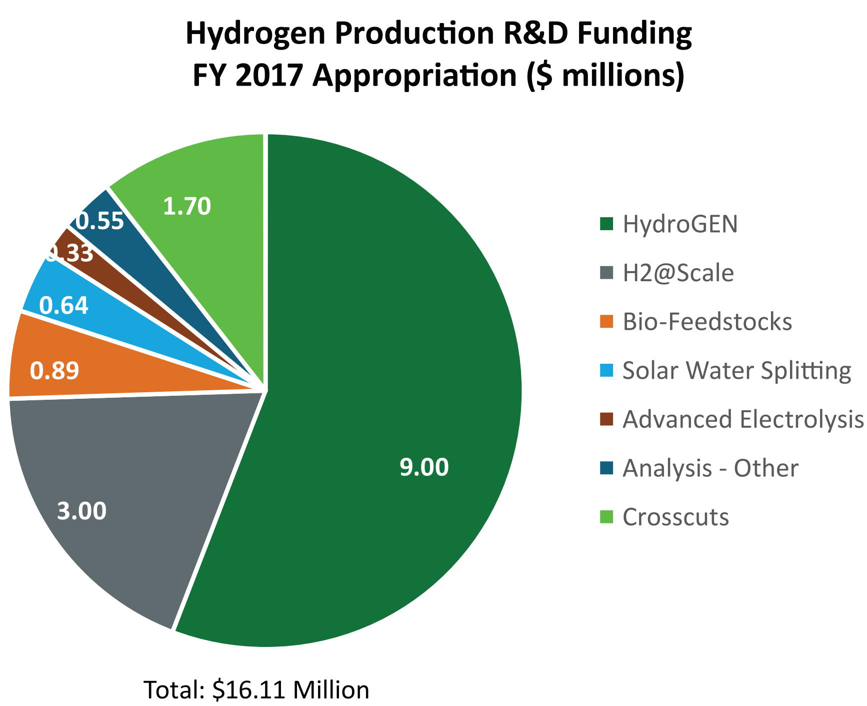

FIGURE 2. FY 2017 Appropriations

UPCOMING ACTIVITIES AND PLANS

Future plans for the Hydrogen Production sub-program include:

- Continued support of foundational research needs in hydrogen production identified through H2@Scale efforts, including a continued emphasis on research innovations for enhancing efficiency and durability and reducing costs in materials systems for all hydrogen production pathways.
- Expanded early-stage R&D through the HydroGEN Advanced Water Splitting Materials Consortium, including initiation of the 19 projects selected in the FY 2017 funding opportunity announcement and ongoing enhancement of the HydroGEN national laboratory core capabilities in advanced electrochemical, PEC, and thermochemical water splitting.

- Expanded emphasis on the development of robust materials characterization protocols and performance benchmarking standards to verify the potential of materials innovations.
- Continued leveraging of cross-office and cross-agency R&D opportunities and resources, including expanded collaboration with the National Science Foundation, the DOE Office of Basic Energy Sciences, and Advanced Research Projects Agency-Energy.

Future activities are subject to appropriations.

Eric Miller
Hydrogen Production and Delivery Program 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