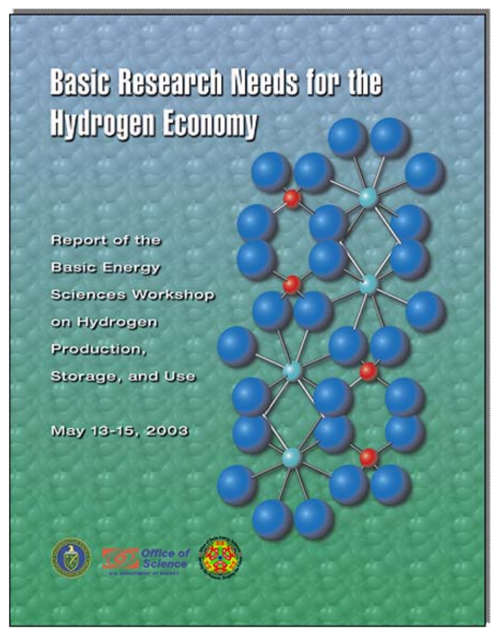
II Basic Research

The Basic Energy Sciences (BES) office within the DOE Office of Science supports the DOE Hydrogen Program by providing basic, fundamental research in those technically challenging areas facing the Program, complementing the applied research and demonstration projects conducted by the Offices of Energy Efficiency and Renewable Energy; Fossil Energy; and Nuclear Engineering, Science and Technology. In May 2005 Secretary of Energy Samuel W. Bodman announced the selection of over $64 million in BES research and development projects aimed at making hydrogen fuel cell vehicles and refueling stations available, practical and affordable for American consumers by 2020.

A total of 70 hydrogen research projects were selected to focus on fundamental science and enable revolutionary breakthroughs in hydrogen production and storage, in addition to new fuel cell technologies. Participants in the projects include more than 50 research organizations in 25 states. The organizations include academic institutions, industry, and national laboratories.

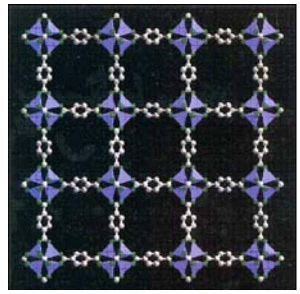
The projects address five technical focus areas identified during the Department of Energy's May 2003 workshop on "Basic Research Needs for the Hydrogen Economy." The key finding of that workshop was summarized as follows: *"Bridging the gaps that separate the hydrogen- and fossil-fuel based economies in cost, performance, and reliability goes far beyond incremental advances in the present state of the art. Rather, fundamental breakthroughs are needed in the understanding and control of chemical and physical processes involved in the production, storage, and use of hydrogen. Of particular importance is the need to understand the atomic and molecular processes that occur at the interface of hydrogen with materials in order to develop new materials suitable for use in a hydrogen economy. New materials are needed for membranes, catalysts, and fuel cell assemblies that perform at much higher levels, at much lower cost, and with much longer lifetimes. Such breakthroughs will require revolutionary, not evolutionary, advances. Discovery of new materials, new chemical processes, and new synthesis techniques that leapfrog technical barriers is required. This kind of progress can be achieved only with highly innovative, basic research."*

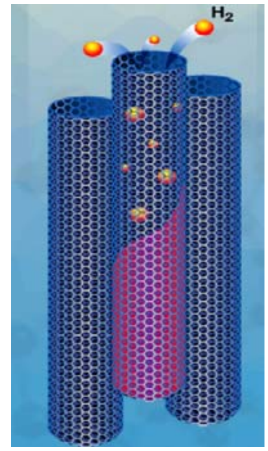


The BES initiatives are part of a comprehensive, balanced portfolio of basic and applied research, technology development, and learning demonstration projects aimed to significantly advance President Bush's Hydrogen Fuel Initiative. The projects were selected through an open, merit-reviewed, competitive solicitation process. The $64 million will be provided to the awardees by the Department over three years, subject to Congressional appropriations.

Following are brief descriptions of the five technical areas addressed by the BES program, along with the project titles and organizations of the 70 awards.

A. Novel Materials for Hydrogen Storage (17 projects, $19.8 million over three years)





On-board hydrogen storage has been identified by both the National Academy of Sciences and the DOE as a key technology for the successful implementation of a hydrogen economy. However, significant scientific challenges remain, highlighting the need for further basic research. Within the hydrogen storage topic, 17 projects will be awarded to 10 universities and 6 national laboratories (Table 1). A broad range of research in hydrogen storage is covered by these selected projects, including complex hydrides; nanostructured and novel materials; theory, modeling, and simulation; and state-of-the-art analytical and characterization tools to develop novel storage materials and methods.

Table 1. Novel Hydrogen Storage Materials

Institution	Project Title
Massachusetts Institute of Technology	Theory and Modeling of Materials for Hydrogen Storage
Washington University	*In Situ* NMR Studies of Hydrogen Storage Systems
University of Pennsylvania	Chemical Hydrogen Storage in Ionic Liquid Media
Colorado School of Mines	Molecular Hydrogen Storage in Novel Binary Clathrate Hydrates at Near-Ambient Temperatures and Pressures
Georgia Institute of Technology	First-Principles Studies of Phase Stability and Reaction Dynamics in Complex Metal Hydrides
Louisiana Tech University	Understanding the Local Atomic-Level Effect of Dopants In Complex Metal Hydrides Using Synchrotron X-ray Absorption Spectroscopy and Density Functional Theory
University of Missouri, Rolla	In-Situ Neutron Diffraction Studies of Novel Hydrogen Storage Materials
University of Georgia	Integrated Nanoscale Metal Hydride-Catalyst Architectures for Hydrogen Storage
Tulane University	Molecular Design Basis for Hydrogen Storage in Clathrate Hydrates
Southern Illinois University	First Principles Based Simulation of Hydrogen Interactions in Complex Hydrides
Massachusetts Institute of Technology	High Throughput Screening of Nanostructured Hydrogen Storage Materials
Pacific Northwest National Laboratory	Control of Hydrogen Release and Uptake in Condensed Phases
Brookhaven National Laboratory	Atomistic Transport Mechanisms in Reversible Complex Metal Hydrides
Ames Laboratory	Complex Hydrides - A New Frontier for Future Energy Applications
Lawrence Berkeley National Laboratory	A Synergistic Approach to the Development of New Classes of Hydrogen Storage Materials
Oak Ridge National Laboratory	Atomistic Mechanisms of Metal-Assisted Hydrogen Storage in Nanostructured Carbons
Savannah River National Laboratory	Elucidation of Hydrogen Interaction Mechanisms with Metal-Doped Carbon Nanostructures

B. Membranes for Separation, Purification, and Ion Transport (16 projects, $12.3 million over three years)

Novel membranes are needed to selectively transport atomic, molecular, or ionic hydrogen and oxygen for hydrogen production and fuel cell applications. The 16 projects selected, which include 13 universities and 3 national laboratories, address integrated nanoscale architectures; fuel cell membranes; and theory, modeling, and simulation of membranes and fuel cells (Table 2).

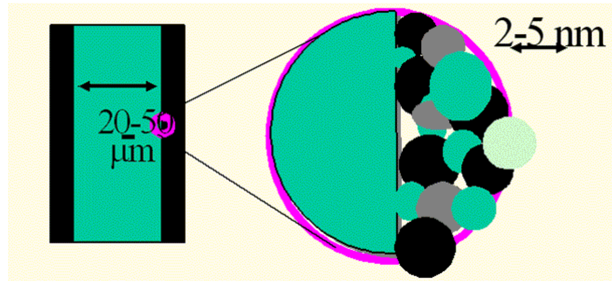
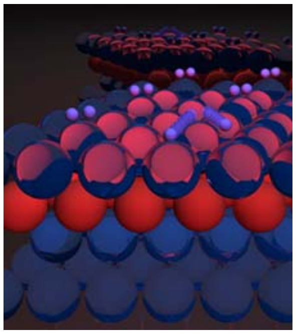
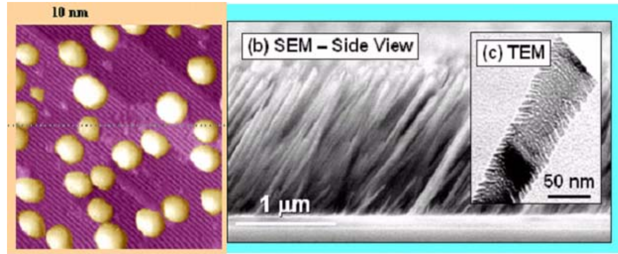


Table 2. Membranes for Separation, Purification, and Ion Transport

Institution	Project Title
University of Utah	Computer Simulation of Proton Transport in Fuel Cell Membranes
Clemson University	New Proton-Conducting Fluoropolymer Electrolytes for PEM Fuel Cells
Carnegie Mellon University	Rapid Ab Initio Screening of Ternary Alloys for Hydrogen Production
Rensselaer Polytechnic Institute	Sol-Gel Based Polybenzimidazole Membranes for Hydrogen Pumping Devices
Lehigh University	Porous and Glued Langmuir-Blodgett Membranes
University of Pennsylvania	The Development of Nano-Composite Electrodes for Natural Gas-Assisted Steam Electrolysis for Hydrogen Production
Case Western Reserve University	Theory, Modeling, and Simulation of Ion Transport in Ionomer Membranes
University of Tennessee	A Unified Computational, Theoretical, and Experimental Investigation of Proton Transport through the Electrode/Electrolyte Interface of Proton Exchange Membranes Fuel Cells Systems
Vanderbilt University	Template-Assisted Fabrication of Well-Defined Diffusion/Catalyst/Ionomer Networks
California Institute of Technology	Polymer Functionalized Zeolite Proton Exchange Membranes (PFZ-PEM) for Medium Temperature (<299°C) Fuel Cells
University of Rochester	Composite Fuel Cell Membranes Containing Aligned Inorganic Particles
University of North Carolina, Chapel Hill	Proton Exchange Membranes for Next Generation Fuel Cells
Cornell University	Novel Intermetallic Catalysts to Enhance PEM Membrane Durability
Lawrence Berkeley National Laboratory	Nanocomposite Proton Conductor
Los Alamos National Laboratory	Fundamentals of Hydroxide Conducting Systems for Fuel Cells and Electrolyzers
Pacific Northwest National Laboratory	Charge Transfer, Transport, and Reactivity in Complex Molecular Environments: Theoretical Studies for the Hydrogen Fuel Initiative

C. Catalyst Design at the Nanoscale (18 projects, $15.8 million over three years)





Catalysis plays a vital role in hydrogen production, storage and use. Specifically, catalysts are needed for converting solar energy to chemical energy, producing hydrogen from water or carbon-containing fuels such as coal and biomass, increasing efficiency in hydrogen storage kinetics, and producing electricity from hydrogen in fuel cells. Nanoscale catalyst designs will be explored through 18 projects involving 12 universities and 5 national laboratories (Table 3). Research areas include innovative synthetic techniques; novel characterization techniques; and theory, modeling, and simulation of catalytic pathways.

Table 3. Catalyst Design at the Nanoscale

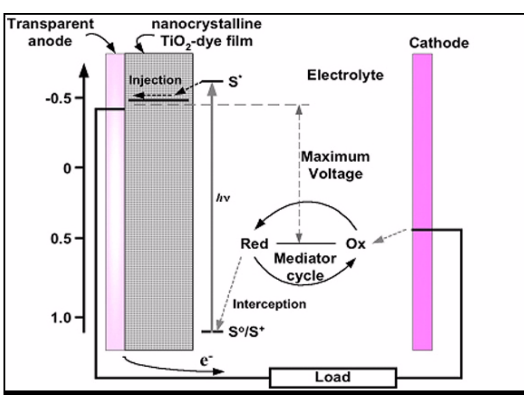
Institution	Project Title
University of Pittsburgh	Multiscale Tailoring of Highly Active and Stable Nanocomposite Catalysts
Tufts University	Nanostructured, Metal-Ion Modified Ceria and Zirconia Oxidation Catalysts
Massachusetts Institute of Technology	Instability of Noble Metal Catalysts in Proton Exchange Membrane Fuel Cells: Experiments and Theory
University of Wisconsin	Atomic-Scale Design of a New Class of Alloy Catalysts for Reactors Involving Hydrogen: A Theoretical and Experimental Approach
University of California, Santa Barbara	Nanostructured Metal Carbide Catalysts for the Hydrogen Economy
University of Wyoming	eNMR for In-Situ Fuel Cell Catalyst Characterization
Yale University	Novel Reforming Catalysts
Texas A&M University	Theory-Guided Design of Nanoscale Multi-Metallic Catalysts for Fuel Cells
Johns Hopkins University	Nanoengineered Mesoporous Metals with Monolayer Thick Precious Metal Catalyst Skin
University of Illinois	Reversible Dehydrogenation of Boron Nanoclusters
Texas Tech University	Strategies for Probing Nanometer-Scale Electrocatalysts: From Single Particles to Catalyst-Membrane Architectures
Arizona State University	A Surface Stress Paradigm for Studying and Developing Catalyst and Storage Materials Relevant to the Hydrogen Economy
University of Illinois	Cathode Catalysis in Hydrogen/Oxygen Fuel Cells
Argonne National Laboratory	Fundamental Studies of Electrocatalysis for Low Temperature Fuel Cell Cathodes
Stanford Linear Accelerator Center	Development and Mechanistic Characterization of Alloy Fuel Cell Catalysts
Brookhaven National Laboratory	Metal Oxide-Supported Platinum Monolayer Electrocatalysts for Oxygen Reduction
Sandia National Labs- Albuquerque	Design of Novel Nano-Catalysts for Improved Hydrogen Production
Oak Ridge National Laboratory	Nanoscale Building Blocks for Multi-Electron Electrocatalysis: The Oxygen Reduction Reaction in Fuel Cells and Oxygen Evolution in Water Electrolysis

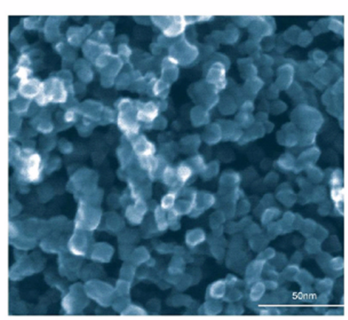
D. Solar Hydrogen Production (13 projects, $10 million over three years)

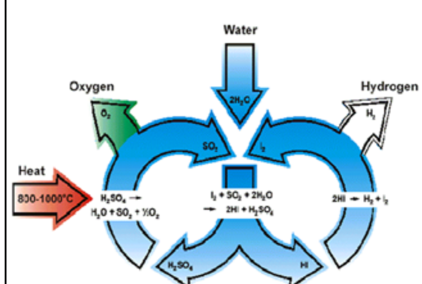
Efficient and cost-effective conversion of sunlight to hydrogen by splitting water is a major enabling technology for a viable hydrogen economy. Hydrogen production via solar energy conversion will be studied through 13 projects at 8 universities, 1 industry company, and 3 national laboratories (Table 4). The projects address nanoscale structures; inorganic and organic semiconductors and other high-performance materials; and theory, modeling, and simulation of photochemical processes.

Table 4. Solar Hydrogen Production

Institution	Project Title
Colorado State University	A Combinatorial Approach to Realization of Efficient Water Photoelectrolysis
California Institute of Technology	Sunlight-Driven Hydrogen Formation by Membrane-Supported Photoelectrochemical Water Splitting
University of Arizona	"Electrochemically Wired" Dye-Modified Dendrimers and Semiconductor Nanoparticles in Sol-Gel Thin Films: Toward Vectorial Electron Transport in Hybrid Materials and Solar-Assisted Hydrogen Production
University of California, Santa Cruz	Hydrogen Generation Using Integrated Photovoltaic and Photoelectrochemical Cells
Pennsylvania State University	Dye-Sensitized Tandem Photovoltaic Cells
Purdue University	Biomineralization Inspired Electrochemical Fabrication of High Performance Photoelectrodes for Solar Hydrogen Production
Pennsylvania State University	Photoelectrochemistry of Semiconductor Nanowire Arrays
University of Washington	Real-Time Atomistic Simulation of Light Harvesting and Charge Transport for Solar Hydrogen Production
Nanoptek Corporation	Bandgap Tailoring of Thin-Film Photocatalysts by Coating onto Stress-Inducing Nanostructured Templates
Virginia Polytechnic Institute and State University	Photoinitiated Electron Collection in Mixed-Metal Supramolecular Complexes: Development of Photocatalysts for Hydrogen Production
Brookhaven National Laboratory	Catalyzed Water Oxidation by Solar Irradiation of Band-Gap-Modified Semiconductors
Pacific Northwest National Laboratory	Fundamental Investigations of Water Splitting on Model TiO_2 Photocatalysts Doped for Visible Light Absorption
National Renewable Energy Laboratory	Ultra-High Efficiency Solar Hydrogen Production via Singlet Fission in Molecules and Exciton Multiplication in Quantum Dots







E. Bio-inspired Materials and Processes (6 projects, $7 million over three years)

Fundamental research into the molecular mechanisms underlying biological hydrogen production is the key to our ability to adapt, exploit, and extend what nature has accomplished for our own renewable energy needs. Bio-inspired materials and processes for hydrogen production will be investigated through 6 projects at 5 universities and 1 national laboratory (Table 5). Research includes enzyme catalysis; bio-hybrid energy coupled systems; and theory, modeling, and nanostructure design.

Table 5. Bio-Inspired Materials and Processes

Institution	Project Title
Pennsylvania State University	A Hybrid Biological/Organic Half-Cell for Generating Dihydrogen
University of Washington	Hydrogenases of Methanococcus Maripaludis
North Carolina State University	RNA Mediated Synthesis of Catalysts for Hydrogen Production and Oxidation
University of Georgia	Fundamental Studies of Recombinant Hydrogenases
University of Pennsylvania	Modular Designed Protein Constructions for Solar Generated H_2 from Water
National Renewable Energy Laboratory	Structural, Functional, and Integration Studies of Biocatalysts for Development of Solar Driven, Bio-Hybrid, H_2-Production Systems