

**Department of Energy, Office of Science  
Hydrogen Fuel Initiative  
Basic Energy Sciences, 70 FY 2005 Hydrogen Awards**

Principal Investigator(s)			Proposal Title
Last Name	First Name	Institution	

**Category A: Novel Hydrogen Storage Materials**

A: Novel Hydrogen Storage Materials -- Grant			
Ceder	Gerbrand	Massachusetts Institute of Technology	Theory and Modeling of Materials for Hydrogen Storage
Conradi	Mark S.	Washington University	In Situ NMR Studies of Hydrogen Storage Systems
Sheddon	Larry G.	University of Pennsylvania	Chemical Hydrogen Storage in Ionic Liquid Media
Sloan	E. Dendy	Colorado School of Mines	Molecular Hydrogen Storage in Novel Binary Clathrate Hydrates at Near-Ambient Temperatures and Pressures
Chou	Mei-Yin	Georgia Institute of Technology	First-Principles Studies of Phase Stability and Reaction Dynamics in Complex Metal Hydrides
Dobbins	Tabbatha	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
Yelon	William B.	University of Missouri, Rolla	In-Situ Neutron Diffraction Studies of Novel Hydrogen Storage Materials
Zhao	Yiping	University of Georgia	Integrated Nanoscale Metal Hydride-Catalyst Architectures for Hydrogen Storage
John	Vijay, T.	Tulane University	Molecular Design Basis for Hydrogen Storage in Clathrate Hydrates
Ge	Qingfeng	Southern Illinois University	First Principles Based Simulation of Hydrogen Interactions in Complex Hydrides
Chen	Gang	Massachusetts Institute of Technology	High Throughput Screening of Nanostructured Hydrogen Storage Materials
A: Novel Hydrogen Storage Materials -- Laboratory			
Autrey	Tom	Pacific Northwest National Laboratory	Control of Hydrogen Release and Uptake in Condensed Phases
Sutter/Vogt	Peter/Tom	Brookhaven National Laboratory	Atomistic Transport Mechanisms in Reversible Complex Metal Hydrides
Pecharsky	Vitalij	Ames Laboratory	Complex Hydrides - A New Frontier for Future Energy Applications
Long	Jeffrey R.	Lawrence Berkeley National Laboratory	A Synergistic Approach to the Development of New Classes of Hydrogen Storage Materials
Gallego	Nidia C.	Oak Ridge National Laboratory	Atomistic Mechanisms of Metal-Assisted Hydrogen Storage in Nanostructured Carbons
Zidan	Ragaiy	Savannah River National Laboratory	Elucidation of Hydrogen Interaction Mechanisms with Metal-Doped Carbon Nanostructures

**Category B: Membranes for Separation, Purification, and Ion Transport**

B: Membranes for Separation, Purification, and Ion Transport -- Grant			
Voth	Gregory A.	University of Utah	Computer Simulation of Proton Transport in Fuel Cell Membranes
Creager	Stephen E	Clemson University	New Proton-Conducting Fluoropolymer Electrolytes for PEM Fuel Cells
Sholl	David S.	Carnegie Mellon University	Rapid Ab Initio Screening of Ternary Alloys for Hydrogen Production
Benicewicz	Brian C.	Rensselaer Polytechnic Institute	Sol-Gel Based Polybenzimidazole Membranes for Hydrogen Pumping Devices
Regen	Steven L.	Lehigh University	Porous and Glued Langmuir-Blodgett Membranes
Gorte	Raymond J.	University of Pennsylvania	The Development of Nano-Composite Electrodes for Natural Gas-Assisted Steam Electrolysis for Hydrogen Production

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Taylor	Philip L.	Case Western Reserve University	Theory, Modeling, and Simulation of Ion Transport in Ionomer Membranes
Keffer	David J.	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
Jennings	G. Kane	Vanderbilt University	Template-Assisted Fabrication of Well-Defined Diffusion/Catalyst/Ionomer Networks
Goddard III	William, A.	California Institute of Technology	Polymer Functionalized Zeolite Proton Exchange Membranes (PFZ-PEM) for Medium Temperature (<299C) Fuel Cells
Yates	Matthew, Z.	University of Rochester	Composite Fuel Cell Membranes Containing Aligned Inorganic Particles
DeSimone	Joseph M.	University of North Carolina, Chapel Hill	Proton Exchange Membranes for Next Generation Fuel Cells
DiSalvo	Francis	Cornell University	Novel Intermetallic Catalysts to Enhance PEM Membrane Durability

**B: Membranes for Separation, Purification, and Ion Transport -- Laboratory**

De Jonghe	Lutgard C.	Lawrence Berkeley National Laboratory	Nanocomposite Proton Conductor
Pivovar	Bryan, S.	Los Alamos National Laboratory	Fundamentals of Hydroxide Conducting Systems for Fuel Cells and Electrolyzers
Dupuis	Michel	Pacific Northwest National Laboratory	Charge Transfer, Transport, and Reactivity in Complex Molecular Environments: Theoretical Studies for the Hydrogen Fuel Initiative

**Category C: Catalyst Design at the Nanoscale**

**C: Catalyst Design at the Nanoscale -- Grant**

Veser	Gotz	University of Pittsburgh	Multiscale Tailoring of Highly Active and Stable Nanocomposite Catalysts
Flytzani-Stephanopoulos	Maria	Tufts University	Nanostructured, Metal-Ion Modified Ceria and Zirconia Oxidation Catalysts
Shao-Horn	Yang	Massachusetts Institute of Technology	Instability of Noble Metal Catalysts in Proton Exchange Membrane Fuel Cells: Experiments and Theory
Mavrikakis	Emmanoul	University of Wisconsin	Atomic-Scale Design of a New Class of Alloy Catalysts for Reactors Involving Hydrogen: A Theoretical and Experimental Approach
Seshadri	Ram	University of California, Santa Barbara	Nanostructured Metal Carbide Catalysts for the Hydrogen Economy
Buttry	Daniel A.	University of Wyoming	eNMR for In-Situ Fuel Cell Catalyst Characterization
Pfefferle	Lisa	Yale University	Novel Reforming Catalysts
Balbuena	Perla B.	Texas A&M University	Theory-Guided Design of Nanoscale Multi-Metallic Catalysts For Fuel Cells
Erlebacher	Jonah	Johns Hopkins University	Nanoengineered Mesoporous Metals with Monolayer Thick Precious Metal Catalyst Skin
Trenary	Michael	University of Illinois	Reversible Dehydrogenation of Boron Nanoclusters
Korzeniewski	Carol	Texas Tech University	Strategies for Probing Nanometer-Scale Electrocatalysts: From Single Particles to Catalyst-Membrane Architectures
Friesen	Cody	Arizona State University	A Surface Stress Paradigm for Studying and Developing Catalyst and Storage Materials Relevant to the Hydrogen Economy
Gewirth	Andrew A.	University of Illinois	Cathode Catalysis in Hydrogen/Oxygen Fuel Cells

**C: Catalyst Design at the Nanoscale -- Laboratory**

You	Hoydoo	Argonne National Laboratory	Fundamental Studies of Electrocatalysis for Low Temperature Fuel Cell Cathodes
Nilsson	Anders	Stanford Linear Accelerator Center	Development and Mechanistic Characterization of Alloy Fuel Cell Catalysts

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Adzic	Radoslav	Brookhaven National Laboratory	Metal Oxide-Supported Platinum Monolayer Electrocatalysts for Oxygen Reduction
Wilcoxon	Jess P.	Sandia National Labs- Albuquerque	Design of Novel Nano-Catalysts for Improved Hydrogen Production
Brown	Gilbert M.	Oak Ridge National Laboratory	Nanoscale Building Blocks for Multi-Electron Electrocatalysis: The Oxygen Reduction Reaction in Fuel Cells and Oxygen Evolution in Water Electrolysis

**Category D: Solar Hydrogen Production**

D: Solar Hydrogen Production -- Grant			
Parkinson	Bruce	Colorado State University	A Combinatorial Approach to Realization of Efficient Water Photoelectrolysis
Lewis	Nathan S.	California Institute of Technology	Sunlight-Driven Hydrogen Formation by Membrane-Supported Photoelectrochemical Water Splitting
Armstrong	Neal R.	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
Zhang	Jin Z.	University of California, Santa Cruz	Hydrogen Generation Using Integrated Photovoltaic and Photoelectrochemical Cells
Barber	Greg D.	Pennsylvania State University	Dye-Sensitized Tandem Photovoltaic Cells
Choi	Kyoung-Shin	Purdue University	Biomimetic Inspired Electrochemical Fabrication of High Performance Photoelectrodes for Solar Hydrogen Production
Mallouk	Thomas E.	Pennsylvania State University	Photoelectrochemistry of Semiconductor Nanowire Arrays
Prezhdo	Oleg	University of Washington	Real-Time Atomistic Simulation of Light Harvesting and Charge Transport for Solar Hydrogen Production
Guerra	John M.	Nanoptek Corporation	Bandgap Tailoring of Thin-Film Photocatalysts by Coating onto Stress-Inducing Nanostructured Templates
Brewer	Karen J.	Virginia Polytechnic Institute and State University	Photoinitiated Electron Collection in Mixed-Metal Supramolecular Complexes: Development of Photocatalysts for Hydrogen Production
D: Solar Hydrogen Production -- Laboratory			
Fujita	Etsuko	Brookhaven National Laboratory	Catalyzed Water Oxidation by Solar Irradiation of Band-Gap-Modified Semiconductors
Henderson	Michael A.	Pacific Northwest National Laboratory	Fundamental Investigations of Water Splitting on Model TiO <sub>2</sub> Photocatalysts Doped for Visible Light Absorption
Nozik	Art	National Renewable Energy Laboratory	Ultra-High Efficiency Solar Hydrogen Production via Singlet Fission in Molecules and Exciton Multiplication in Quantum Dots

**Category E: Bio-Inspired Materials and Processes**

E. Bio-Inspired Materials and Processes -- Grant			
Golbeck	John H.	Pennsylvania State University	A Hybrid Biological/Organic Half-Cell for Generating Dihydrogen
Leigh	John A.	University of Washington	Hydrogenases of Methanococcus Maripaludis
Feldheim	Daniel L.	North Carolina State University	RNA Mediated Synthesis of Catalysts for Hydrogen Production and Oxidation
Adams	Michael W.W.	University of Georgia	Fundamental Studies of Recombinant Hydrogenases
Dutton	P. Leslie	University of Pennsylvania	Modular Designed Protein Constructions for Solar Generated H <sub>2</sub> From Water
E. Bio-Inspired Materials and Processes -- Laboratory			
Ghirardi	Maria, L.	National Renewable Energy Laboratory	Structural, Functional, and Integration Studies of Biocatalysts for Development of Solar Driven, Bio-Hybrid, H <sub>2</sub> -Production Systems