U.S. DEPARTMENT OF ENERGY | Office of Science

Basic Energy Sciences Overview

Annual Merit Review

Hydrogen & Fuel Cells Program and Vehicle Technologies Program

May 9, 2011

Harriet Kung
Director, Office of Basic Energy Sciences
Office of Science, U.S. Department of Energy

Basic Energy Sciences

Understanding, predicting, and ultimately controlling matter and energy flow at the electronic, atomic, and molecular levels

The Program:

Materials sciences & engineering—exploring macroscopic and microscopic material behaviors and their connections to various energy technologies

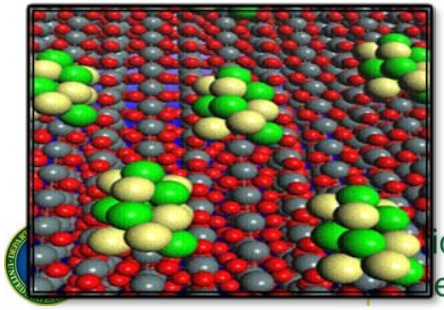
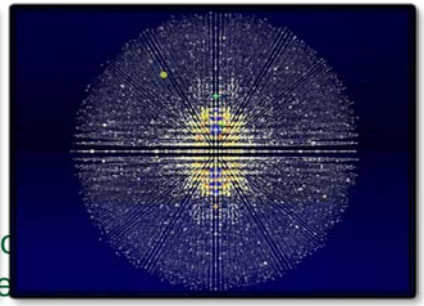
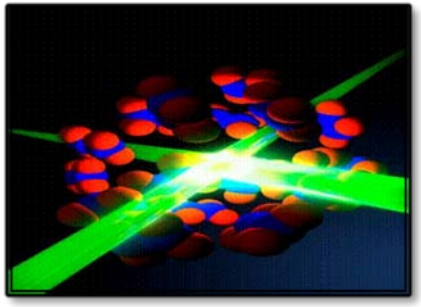
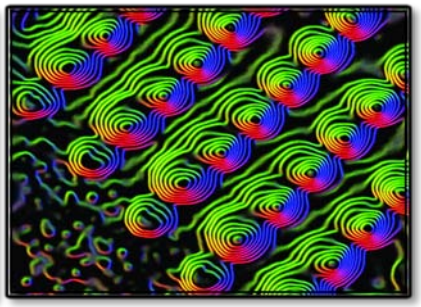
Chemical sciences, geosciences, and energy biosciences—exploring the fundamental aspects of chemical reactivity and energy transduction over wide ranges of scale and complexity and their applications to energy technologies

Supporting:

- 46 Energy Frontier Research Centers
- Solar Fuels Hub
- The largest collection of facilities for electron, x-ray, and neutron scattering in the world

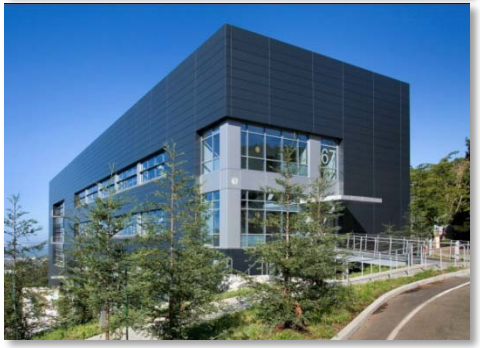
The Scientific Challenges:

- Synthesize, atom by atom, new forms of matter with tailored properties, including nano-scale objects with capabilities rivaling those of living things
- Direct and control matter and energy flow in materials and chemical assemblies over multiple length and time scales
- Explore materials & chemical functionalities and their connections to atomic, molecular, and electronic structures
- Explore basic research to achieve transformational discoveries for energy technologies

Transforming the Discovery Process

- Over the past 2 decades, the U.S. has developed and deployed the world's most powerful collection of research facilities for materials and chemical sciences
  - World-leading x-ray and neutron sources
  - Nanoscale science centers
  - High-performance computers
- For the first time in history, we are able to synthesize, characterize, and model materials and chemical behavior at the length scale where this behavior is controlled
- This transformational leap conveys a significant competitive advantage



FY12 Budget Request: Science for Energy

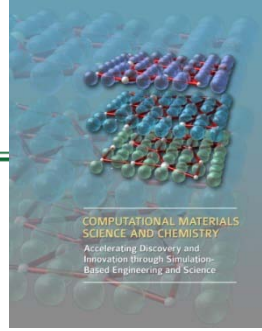
Non-carbon Sources	**(Dollars in thousands)**
Solar Electricity from Photovoltaics	+ 8,000
Advanced Nuclear Energy Systems	+ 8,000
Materials under Extreme Environments	+15,000
Carbon Capture and Sequestration	
Carbon Capture	+ 8,000
Carbon Sequestration	+ 8,000
Transportation and Fuel Switching	
Energy Systems Simulation - Combustion	+ 15,000
Batteries and Energy Storage Hub	+ 34,020
Transmission and Energy Storage	
Electric Power Grid–Enabling Materials Sciences	+ 4,000
Power Electronics	+ 3,500
Batteries and Energy Storage Hub	(same as above)
Efficiency	
Advanced Solid-state Lighting	+ 8,000
Energy Efficiency – Enabling Materials Sciences	+ 4,000

Batteries and Energy Storage Energy Innovation Hub

Transform the Grid and Electrify Transportation

- Improved energy storage is critical for the widespread use of intermittent renewable energy, electric vehicles, and efficient and reliable smart electric grid technologies.
- The Hub, proposed for FY 2012, will develop electrochemical energy storage systems that safely approach theoretical energy and power densities with very high cycle life.
- These are systemic challenges requiring new materials, systems, and knowledge.
- The Hub will address key fundamental questions in energy storage including:
  - Can we approach theoretical energy density?
  - Can we safely increase the rate of energy utilization?
  - Can we create a reversible system with minimal energy loss?
- The Hub will link fundamental science, technology, and end-users, and it will collaborate with relevant Energy Frontier Research Centers, ARPA-E and EERE

Materials and Chemistry by Design

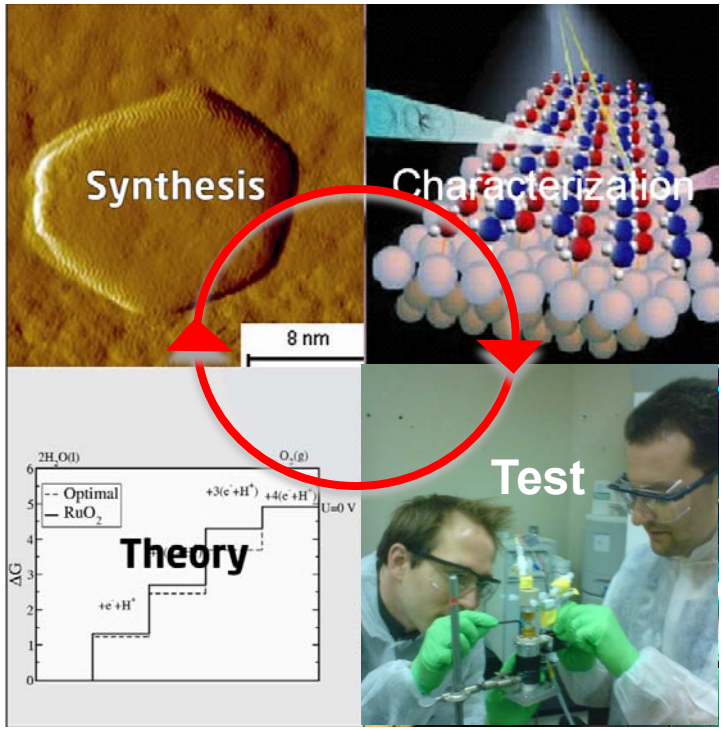


- Research to establish materials design rules to launch an era of predictive modeling, changing the paradigm of materials discovery from serendipity to rational design.
- Discovery of new materials has been the engine driving science frontiers and fueling technology innovations. The U.S. has the world's most powerful suite of tools for materials synthesis, characterization, and computation.
- $40M request to support the following:

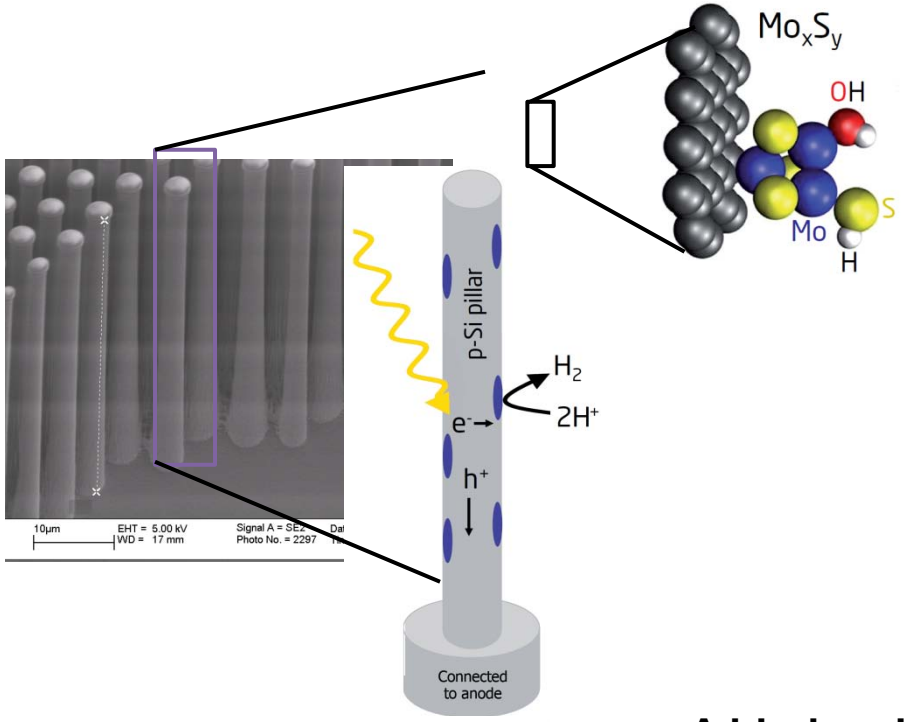
Synthesis: Rational molecular-scale design guided by simulation.

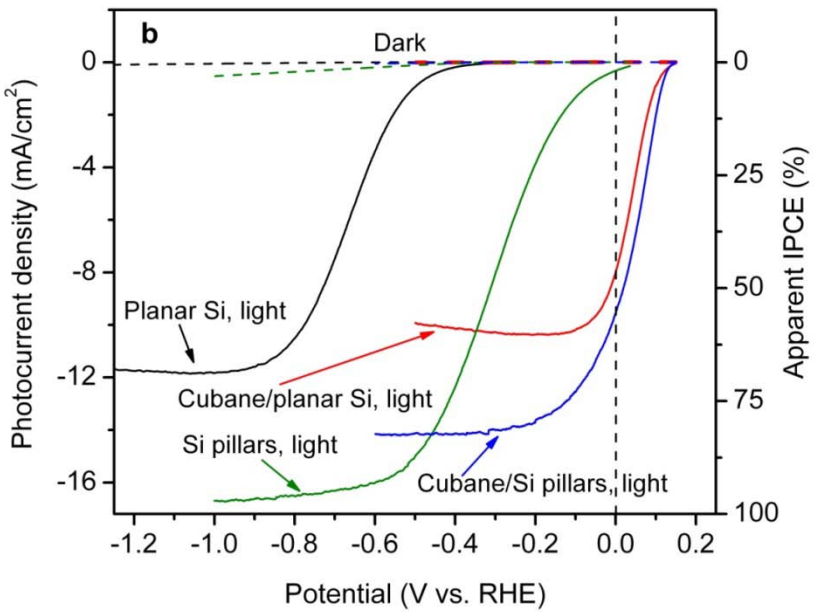
Characterization and Testing: Verify & validate computational designs and software, including in situ measurements using x-ray, neutron, microscopy, and nanoscience facilities.

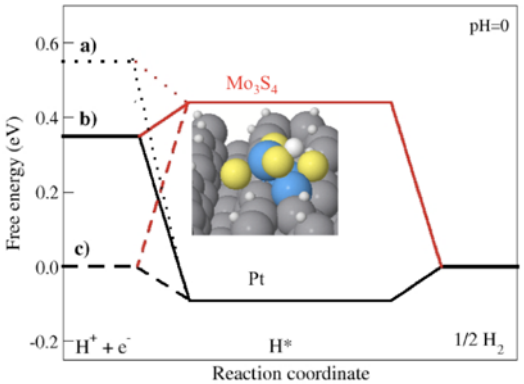
Theory/Simulation: New methods and algorithms for complex, multi-scale systems. Development of software and toolkits through a networked, broad community. Emphasis areas include: catalysis, light-weight materials, and materials for energy applications including radiation-resistant materials, carbon capture, batteries, liquid fuels, and photocatalysis.



Simulation accelerates the discovery of a new catalyst for photo-chemical hydrogen production







- **A bio-inspired catalyst made of earth-abundant Mo_3S_4 clusters efficiently catalyzes water splitting to produce hydrogen when coupled to a p-type Si semiconductor that harvests red photons from the solar spectrum.**
- **Advanced density functional calculations initially suggested MoS_x as potential catalysts, and provided key insights into the nature of the active site.**

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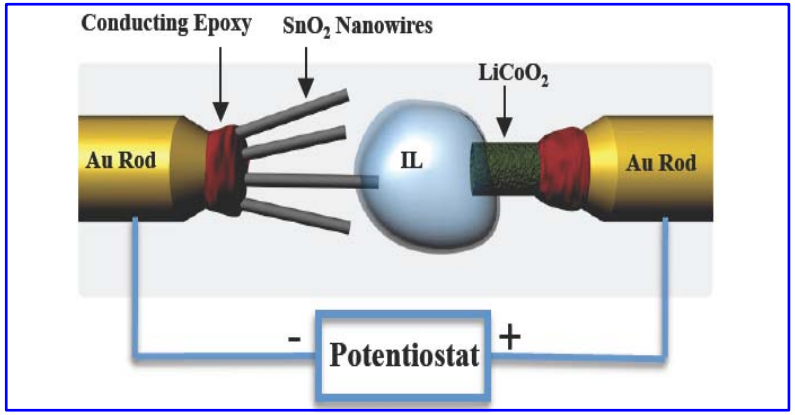
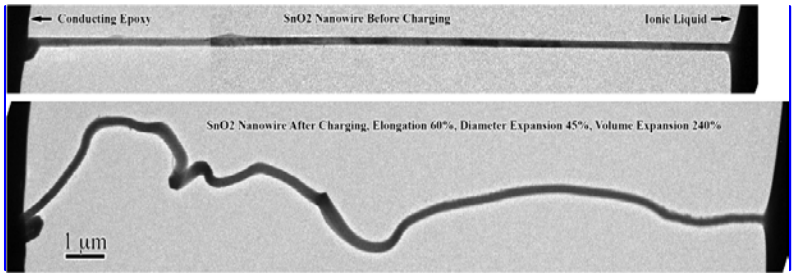
J. Norskov and co-workers
Nature Materials, 24 APRIL 2011
DOI: 10.1038/NMAT3008

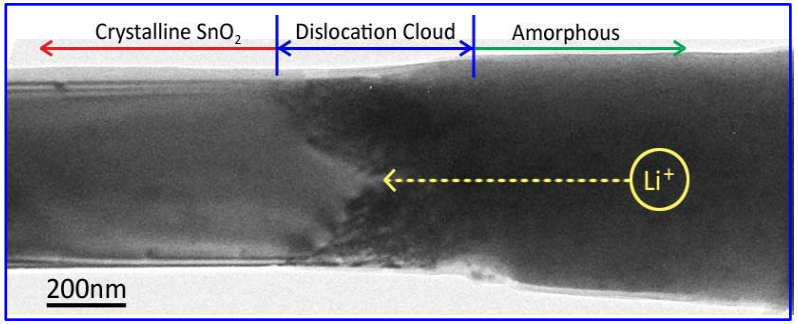
SLAC NATIONAL ACCELERATOR LABORATORY

EFRC Research Reveals Unusual Nanowire Behavior in Battery

- World's smallest battery placed inside an electron microscope yields images of electrochemistry at atomic scales
- New insight into electrochemical processes at the nanoscale:
  - Nanowires can sustain large stresses (>10 GPa) caused by Li^+ transport without breaking—good candidate for battery
  - Elongation and twisting of nanowires during charging may lead to a short circuit and failure of the battery, a key factor to consider during design







Jian Yu Huang, et al., Science 330, 1515 (2010)

Research at SNL supported by the *Center for Science of Precision Multifunctional Nanostructures for Electrical Energy Storage* (an EFRC led by University of Maryland) and in collaboration with PNNL and university contributors

May 25 – 27, 2011, Washington, D.C.

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Renaissance Penn
Quarter Hotel

Science for our Nation's Energy Future

Energy Frontier Research Centers Summit & Forum

Transforming the future of energy and the environment.

Science for Our Nation's Energy Future will:

- Explore the challenges and opportunities in applying America's extraordinary scientific and technical resources to critical energy needs
- Highlight early successes of the Office of Science Energy Frontier Research Centers
- Promote collaboration across the national energy enterprise

Expected Participants include:

- Leaders from science, industry and government from the US and abroad
- Students, young researchers, and senior investigators
- Members of the media and the general public

www.energyfrontier.us

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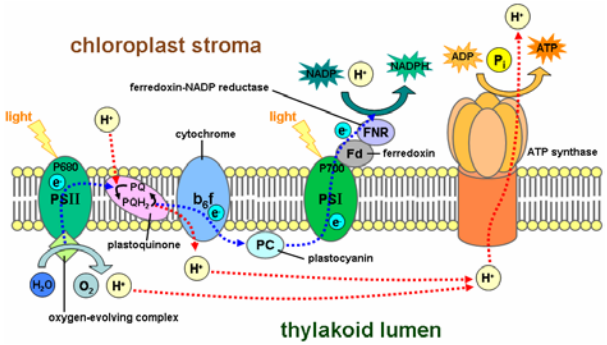
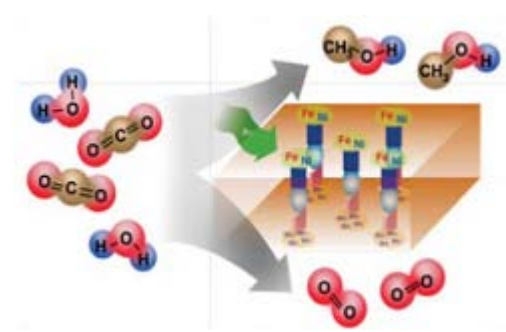
Fuels from Sunlight Energy Innovation Hub:
Joint Center for Artificial Photosynthesis (JCAP)

- The design of highly efficient, non-biological, molecular-level "machines" that generate fuels directly from sunlight, water, and carbon dioxide is the challenge.
- Basic research has provided an understanding of the complex photochemistry of the natural photosynthetic system and the use of inorganic photo-catalytic methods to split water or reduce carbon dioxide – key steps in photosynthesis.
- **JCAP Mission: To demonstrate a scalable, manufacturable solar-fuels generator using Earth-abundant elements, that, with no wires, robustly produces fuel from the sun 10 times more efficiently than (current) crops.**
- JCAP R&D focuses on:
  - Accelerating the rate of catalyst discovery for solar fuel reactions
  - Discovering earth-abundant, robust, inorganic light absorbers with optimal band gap
  - Providing system integration and scale-up
- **Begun in FY 2010, JCAP serves as an integrative focal point for the solar fuels R&D community – formal collaborations have been established with 20 Energy Frontier Research Centers.**



Natural photosynthesis



Artificial photosynthesis

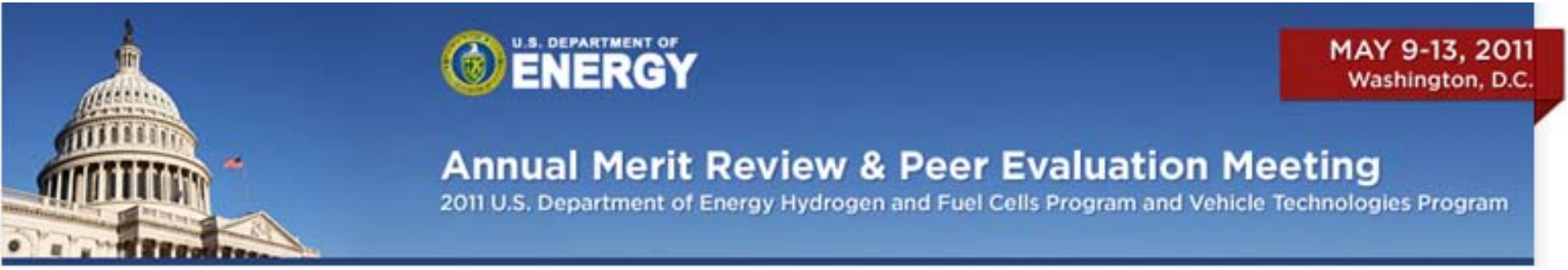
2011 AMR Meeting: BES Hydrogen Production PIs

- 13 Oral Presentations (All BES Talks in Crystal Gateway – Salon V)

Weds Afternoon May 11: 2:15-6:15PM
Talk Numbers: BES001 – BES007

Thurs Morning May 12: 11:30-12:30
Talk Numbers: BES008 – BES009

Thurs Afternoon May 12: 4:15-6:15PM
Talk Numbers: BES0010 – BES013

- 8 Poster Presentations (All in Crystal Gateway – Grand Ballroom)

Weds Evening May 11: 6:30-8:30PM
Poster Numbers: BES014 - BES021