U.S. DEPARTMENT OF ENERGY | Office of Science

Basic Energy Sciences Update

Hydrogen and Fuel Cell Technical Advisory Committee
April 21, 2015

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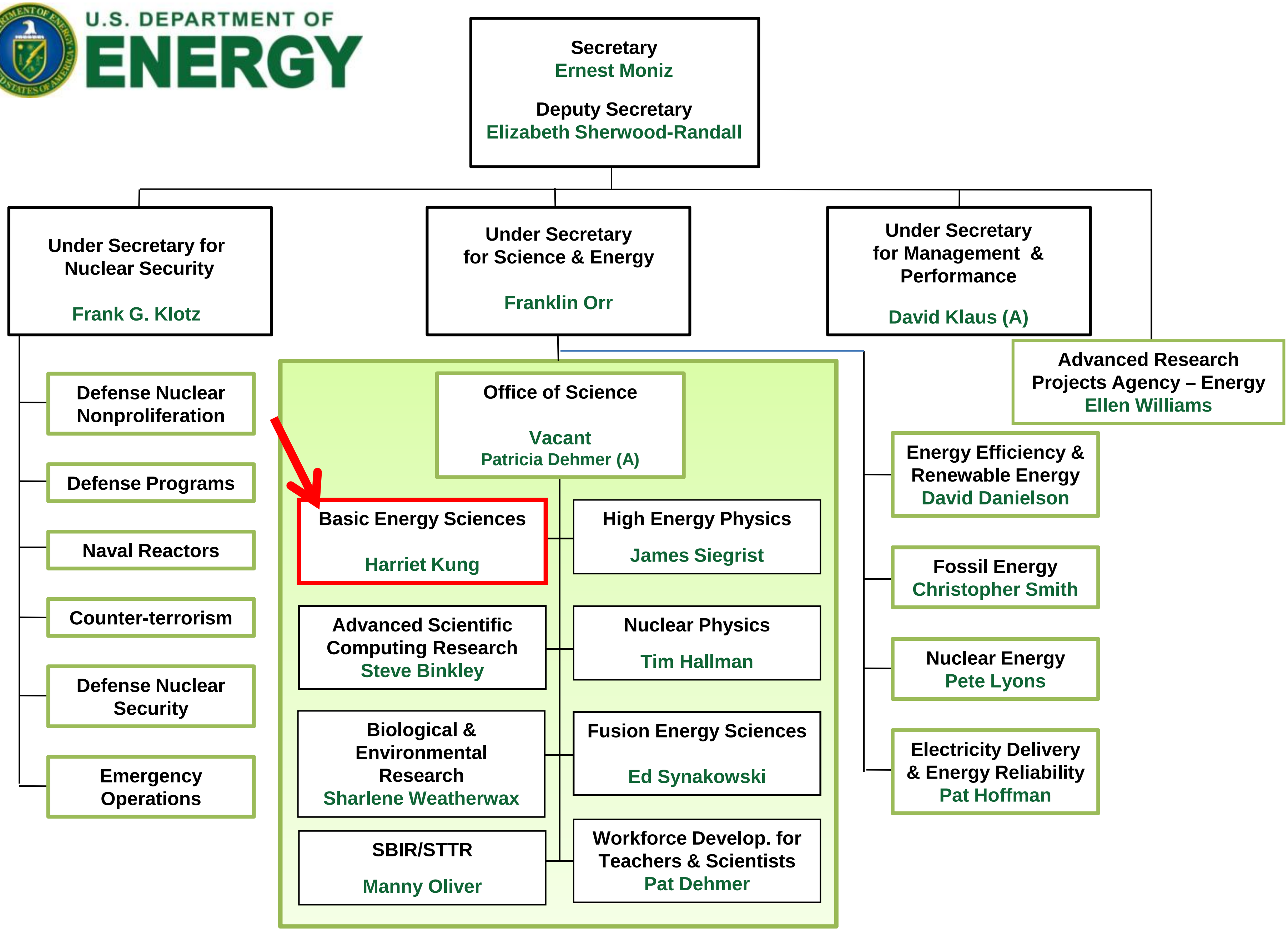
Office of Science, U.S. Department of Energy

U.S. DEPARTMENT OF
ENERGY



Basic Energy Sciences

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

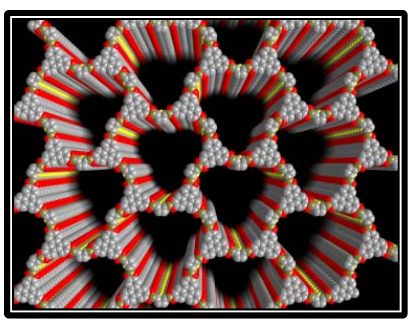
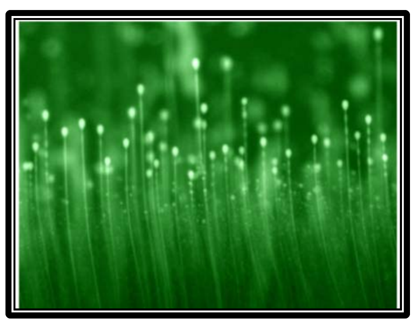
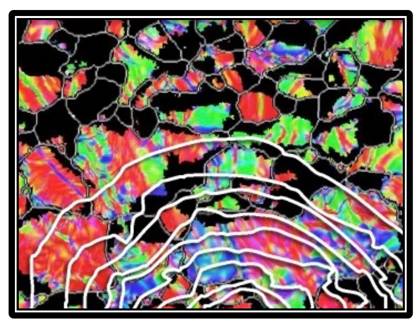
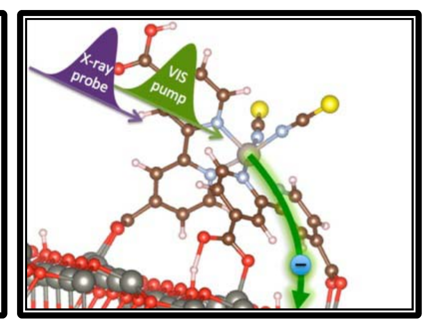
Supporting:

- 32 Energy Frontier Research Centers
- Fuels from Sunlight & Batteries and Energy Storage Hubs
- 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

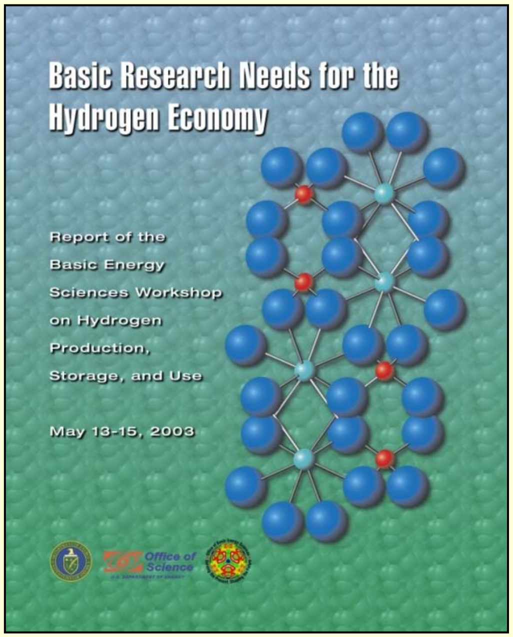
Understanding, predicting, and ultimately controlling matter and energy flow at the electronic, atomic, and molecular levels

BES Strategic Planning and Program Development

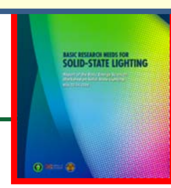
1999 2000 2002 2004 2006 2008 2010 2012 2015

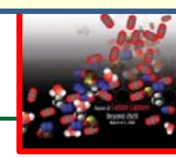
Basic Research R&D Plan: BES Hydrogen Workshop Report

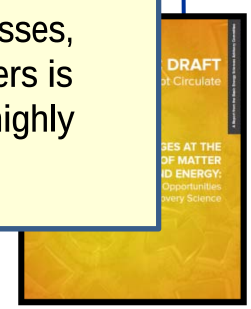


May 13-15, 2003

"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."







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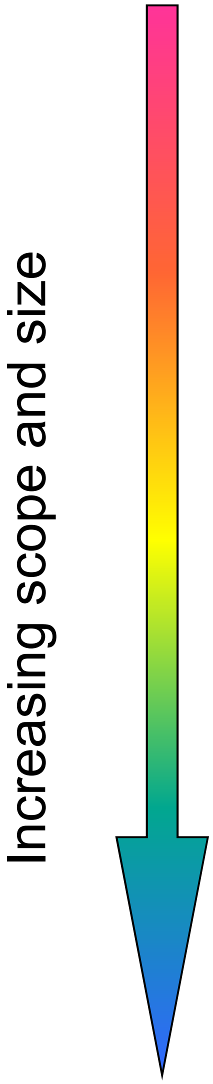
BES

BES Research Activities

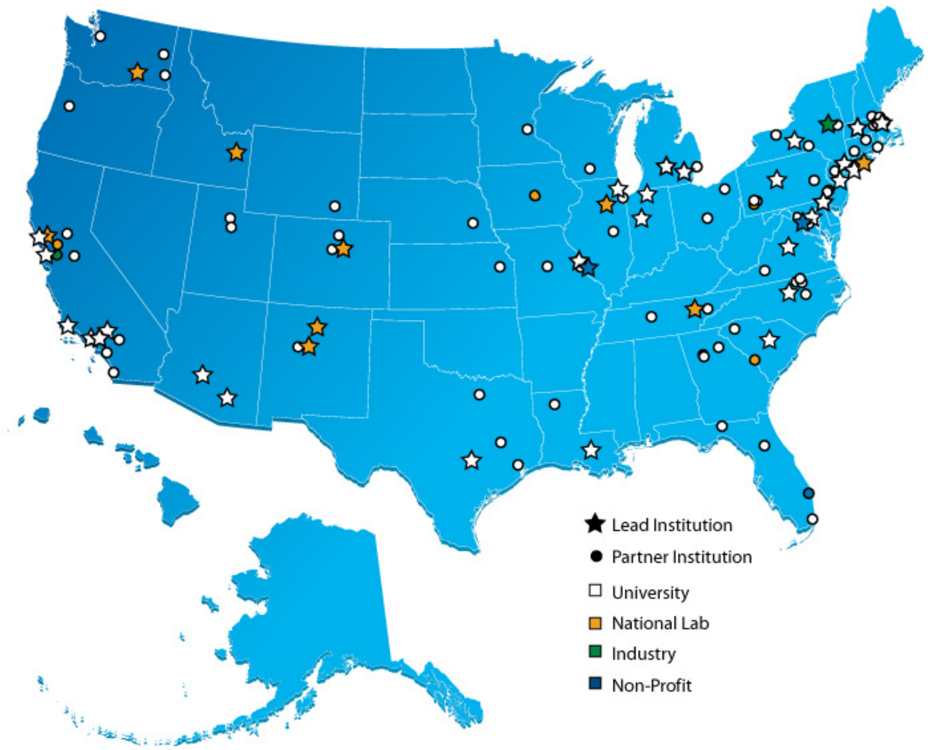


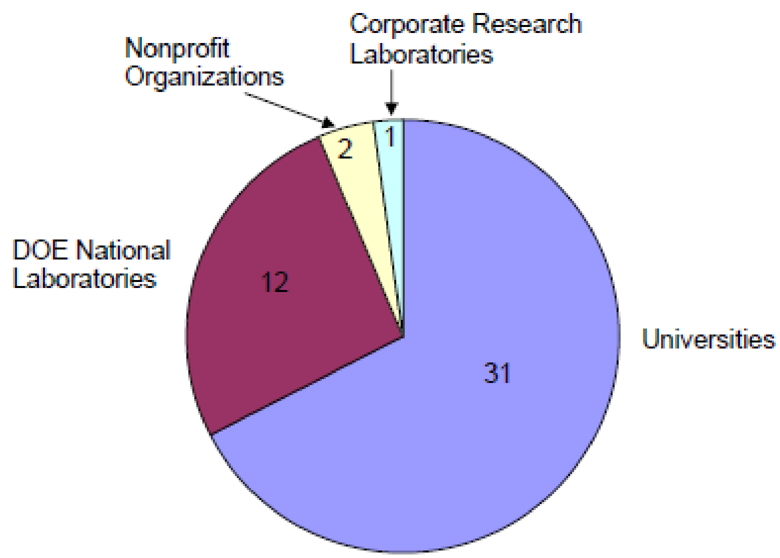
- Core Research (>1,300 projects)
  Single investigators ($150K/year) and small groups ($500K-$2M/year) engage in fundamental research related to any of the BES core research activities. Investigators propose topics of their choosing.

- Energy Frontier Research Centers (32)
  $2-4 million/year research centers for 4 year award terms; focus on fundamental research described in the Basic Research Needs Workshop reports.

- Energy Innovation Hubs (2)
  Research centers, established in 2010 ($15-25 million/year), engage in basic and applied research, including technology development, on a high-priority topic in energy that is specified in detail in an FOA. Project goals, milestones, and management structure are a significant part of the proposed Hub plan.

46 Energy Frontier Research Centers were Awarded in 2009





Lead Institutions

- **$155M/yr** ($100M/yr from BES; $55M/yr from Recovery Act);
- ~**850** senior investigators
- ~**2,000** students, postdoctoral fellows, and technical staff
- ~**115** institutions
- >**260** scientific advisory board members from **13** countries and >**40** companies

Energy Frontier Research Centers Outcomes and Impacts 2009 - 2014

- PUBLICATIONS, PATENTS, …
  - Near 6,000 peer-reviewed publications; >215 pubs in *Science* and *Nature*.
  - ~280 U.S. and 180 foreign patent applications; ~100 patent/invention disclosures, and ~70 licenses

- HIGHLIGHTS:
  - 17 PECASE and 15 DOE Early Career Awards
  - EFRC students and staff now work in:
    - > 300 university faculty and staff positions;
    - > 475 industrial positions;
    - > 200 national labs, government, and non-profit positions
  - ~70 companies have benefited from EFRC research

- Technical summaries are here: http://science.energy.gov/bes/efrc/
- Accomplishments are here: http://science.energy.gov/~/media/bes/efrc/pdf/efrc/ EFRC-Five-Year-Goals-and-Progress-Summaries-2012-05.pdf

Companies that Benefit from EFRC Research

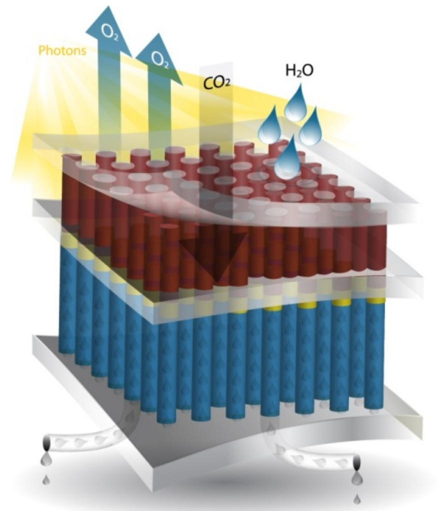
- Alta Devices
- Anellotech
- Caelux Solar Energy
- chromation
- Dioxide Materials
- UbiQD
- Unite to Light
- Synopsys
- Asylum Research, an Oxford Instruments company
- Fulcrum BioEnergy
- electroninks
- ubiquitous energy
- American Aerogel — Revolutionary materials. Superior products.
- amsc
- Samsung Cheil Industries
- Universal Display Corporation
- framergy
- thermoaura
- P&G
- SuperPower Inc. — A Furukawa Company
- Applied Materials
- Philips Lumileds
- iBeam Materials
- Watt Fuel Cell
- HTceramix
- Sigma-Aldrich
- Air Liquide
- ConocoPhillips
- GMZ Energy
- LifeCel Technology
- virdia
- Imperium renewables
- DuPont
- intel
- GE
- GM
- ExxonMobil
- Millifluidica
- Pioneer
- Dow
- Delphi
- Spero — Pioneering A Greener Future
- NanoFlex Power Corporation
- Corning
- Ford
- Toyota
- Gentherm
- Micromidas
- Semprius
- Konica Minolta
- Sharp
- Invista
- NanoIntegris
- SiNode Systems
- Proton OnSite
- Polyera
- Oorja
- LanzaTech
- NanoVoltaics
- Remylop Structured Materials
- QuantumScape
- QD Vision
- Primet Precision Materials
- Orthogonal
- nohms Technologies
- NEXT

Energy Innovation Hubs (Hubs)

HISTORY: An initiative of former Secretary Chu, Hubs address research challenges that have been resistant to solution by conventional R&D management structures.

- ESTABLISHMENT OF HUBS: Proposed throughout the period FY 2010-FY 2014 for initial 5-year terms with the following characteristics:
  - a lead institution with strong scientific leadership;
  - a central location;
  - if geographically distributed, state-of-the-art telepresence technology to enable long distance collaboration;
  - a strong organization and management plan to effect goals.

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



Photoelectrochemical Solar-Fuel Generator

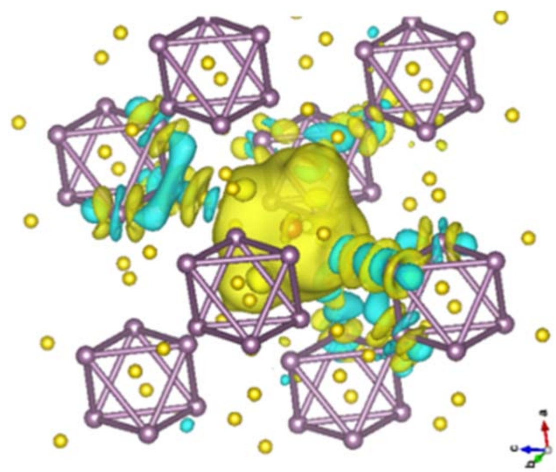
Overview:
- Mission: Develop a solar-fuels generator to produce fuel from the sun 10x more efficiently than crops
- Launched in Sept. 2010 and renewal decision due in Jan. 2015
- Led by Caltech with LBNL as primary partner; additional partners are SLAC, Stanford, UC Berkeley, UC San Diego, UC Irvine
- 2010 - 2015: Development of prototypes capable of efficiently producing hydrogen via photocatalytic water splitting
- 2015**:** Renewal to focus on CO_2 reduction discovery science

Goals and Legacies:
- Library of fundamental knowledge
- Prototype solar-fuels generator
- Science and critical expertise for a solar fuels industry

Renewal Planning:
- Renewal project would restructure R&D to focus primarily on discovery science related to CO_2 reduction for efficient solar-driven production of carbon-based fuels
- Annual funding of up to $15M for a maximum of 5 years reflects reduced project scope
  - De-emphasis of discovery efforts targeted solely towards hydrogen production
  - Development of integrated prototypes mainly to test the capability of new materials, concepts, and/or components
- Renewal decision is expected in April 2015.

Research Accomplishments:
- Discovered method to protect light-absorbing semiconductors (*e.g.* Si, GaAs) from corrosion in basic aqueous solutions while still maintaining excellent electrical charge conduction
- Developed novel high throughput capabilities to prepare and screen light absorbers and electrocatalysts
- Established benchmarking capabilities to compare large quantities of catalysts and light absorbers
- Fabricated and tested integrated artificial photosynthetic prototypes with optimized properties
- Developed new multi-physics modeling tools for analysis of solar-fuels prototypes and processes

Batteries and Energy Storage Hub
Joint Center for Energy Storage Research (JCESR)

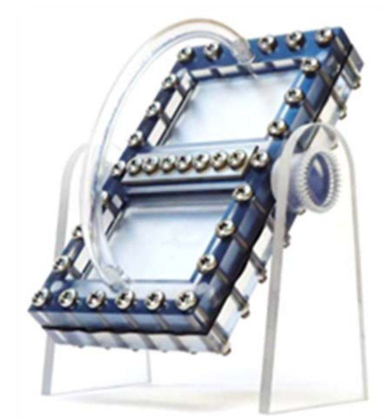


Overview:
- Mission: Discovery Science to enable next generation batteries—beyond lithium ion—and energy storage for transportation and the grid
- Launched in December 2012; Led by George Crabtree (ANL) with national laboratory, university and industrial partners: LBNL, SNL, SLAC, PNNL,UI-UC, NWU, UCh, UI-C, UMich, Dow, AMAT, JCI, CET.

Goals and Legacies:
- 5x Energy Density, 1/5 Cost, Within 5 years
- Library of fundamental knowledge
- Research prototype batteries for grid and transportation
- New paradigm for battery development

FY 2015 - 2016 Milestones:
- For the “electrolyte genome,” calculate data for >10,000 molecular systems.
- Complete techno-economic modeling for electrolyte systems identified by the electrolyte genome, that have the potential to meet the “5-5-5” goals

Research Accomplishments:
- Rational design of high-performance Li_2S cathodes;
- Discovery that incorporation of percolating networks of nanoscale conductors improves charge transfer kinetics in liquid electrodes;
- Techno-economic modeling of alternate designs for lithium-air batteries; Fabrication/testing of the first research prototype Mg-ion battery to establish baseline capability.



Bench-top prototype flow battery

BES Scientific User Facilities

- Available to all researchers ***at no cost*** for non-proprietary research, regardless of affiliation, nationality, or source of research support
- Access based on external peer merit review of brief proposals
- Coordinated access to co-located facilities to accelerate research cycles
- Collaboration with facility scientists an optional potential benefit
- Instrument and technique workshops offered periodically
- A variety of on-line, on-site, and hands-on training available
- Proprietary research may be performed at full-cost recovery

Light Sources

– Advanced Light Source (LBNL)
– Advanced Photon Source (ANL)
– Linac Coherent Light Source (SLAC)
– National Synchrotron Light Source-II (BNL)
– Stanford Synchrotron Radiation Laboratory (SLAC)

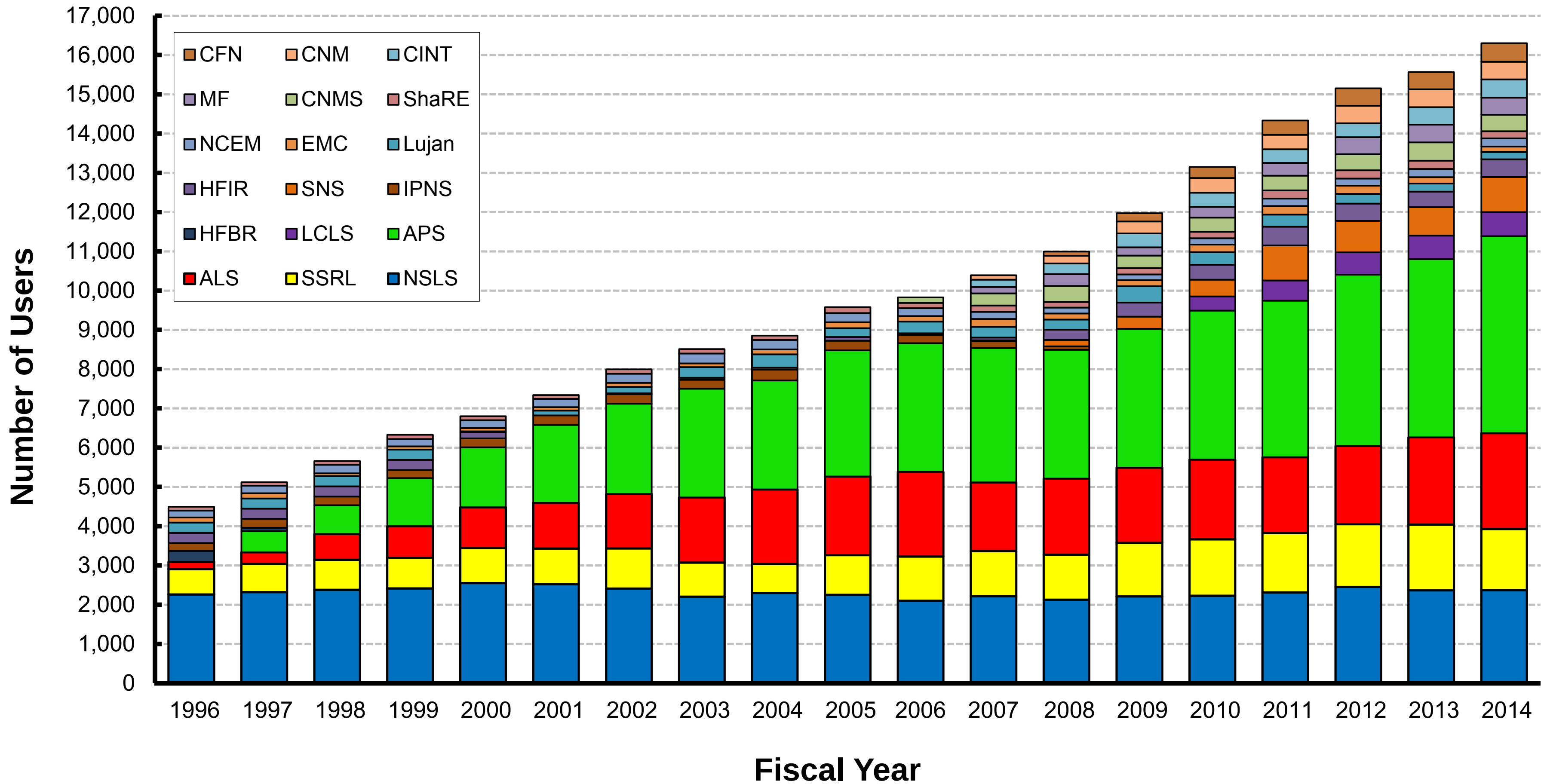
Neutron Sources

– High Flux Isotope Reactor (ORNL)
– Spallation Neutron Source (ORNL

Nanoscale Science Research Centers

– Center for Functional Nanomaterials (BNL)
– Center for Integrated Nanotechnologies (SNL & LANL)
– Center for Nanophase Materials Sciences (ORNL)
– Center for Nanoscale Materials (ANL)
– Molecular Foundry (LBNL)

BES User Facilities Hosted Over 16,000 Users in FY 2014



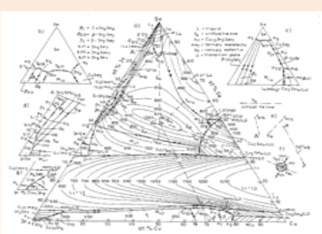
More than 300 companies from various sectors of the manufacturing, chemical, and pharmaceutical industries conducted research at BES scientific user facilities. Over 30 companies were Fortune 500 companies.

Industrial R&D at BES Light Source Facilities

DOW

Solar Shingle

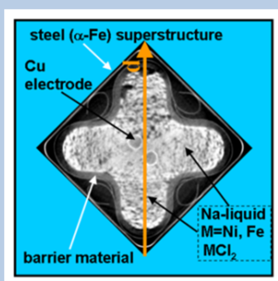
Investigating the process, structure, and property relationships in CuInGaSe (the active material in the first “solar shingles”) with x-ray techniques at synchrotron light sources



GE

Sodium Metal Halide Battery

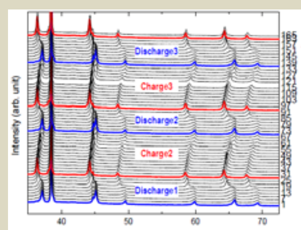
Understanding the distribution of reaction products within the battery to improve the performance using high energy x-ray diffraction



P&G

Lithium Battery

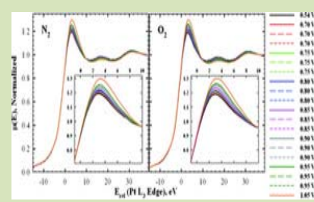
Conducting in situ x-ray diffraction studies at synchrotron light sources to tailor crystal structure of high voltage spinel cathode materials with high capacity and long cycle life



GM

Fuel Cell

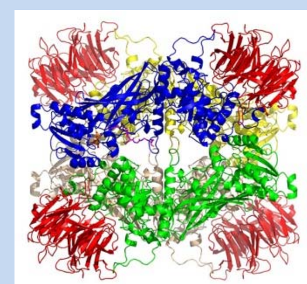
Using x-ray absorption spectroscopy to understand the influences of neighboring oxides on platinum surfaces to obtain vital information on the oxygen reduction reactions in fuel cells



Lilly

From Protein Structures to Drugs

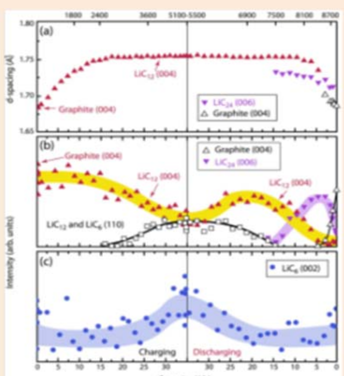
Developing potential life saving drugs by examing the protein structural information, for example, important methylation enzymes that play important roles in cell signaling



Industrial R&D at BES Neutron Scattering Facilities

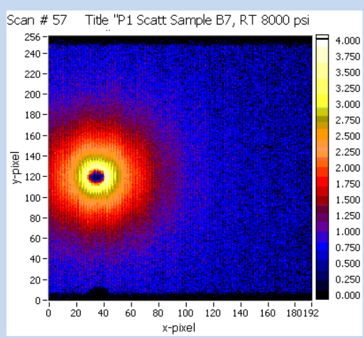
Large-scale Commercial Batteries

Neutron diffraction allowed the study of the structural evolution of large-format commercial batteries under electrochemical cycling to understand failure mechanisms.



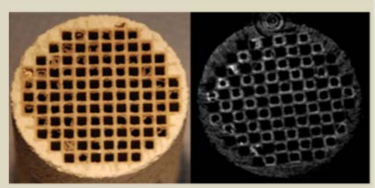
Barnett Shale Deposits

Small Angle Neutron Scattering can examine the size and connectivity of pores in gas-producing shales leading to the development of models of the shale pore accessibility and predicting the value of a shale deposit for producing natural gas.



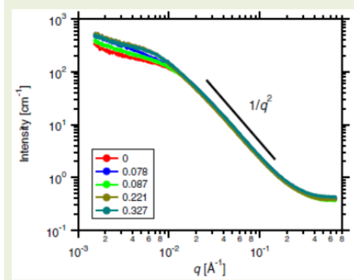
Diesel Fuel Filters

Neutron imaging looks at particulate filters for diesel engines in an effort to improve their performance and fuel efficiency. The technique allows the soot deposition in the filter to be observed directly as in the picture below.



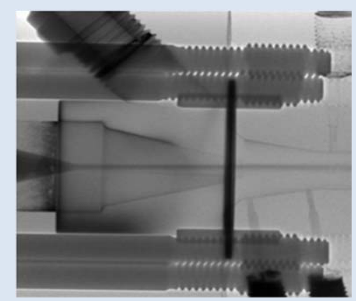
Polymer Nanocomposites

Researchers are using the unique capabilities of neutron scattering to understand the formation, structure, and dynamics of new nanocomposites consisting of complex mixtures of polymers, solvents and inorganic components.



Fluid Flow in Heat Exchange Injectors

The unique sensitivity of neutron imaging for light elements has permitted researchers to observe two-phase fluid flow in heat exchanger injectors for CO_2 refrigerants that promise to reduce global warming without added energy cost.

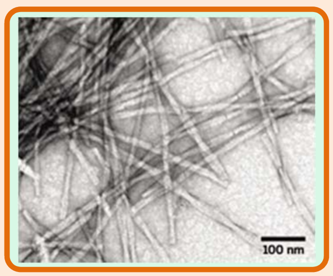


Industry R&D at BES Nano Science Research Centers

NOVARTIS

Disease Therapeutics

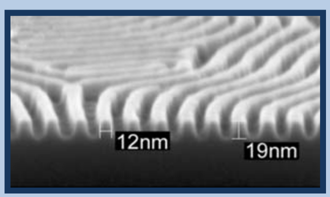
Groundbreaking nanoscience highly sensitive technique for detecting misfolded proteins could help pinpoint Alzheimer's in its early stages and enable researchers to discover new disease therapies.



HGST a Western Digital company

Ultradense Memories

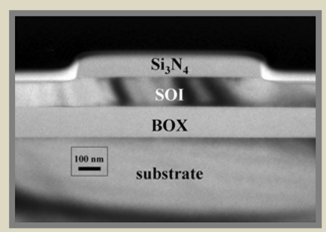
Expertise in polymer nanostructure self-assembly and electron microscopy can be applied to Terabit/cm^2 scale magnetic memories for computing and imaging



IBM

Advanced Microprocessors

Unique hard x-ray Nanoprobe enables nondestructive measure of in-situ strain distributions in silicon-on-insulator (SOI)-based CMOS for sub 130 nm microprocessor technology.



3M

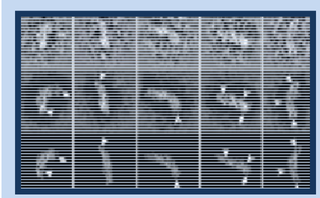
High Performance Fuel Cells

Understanding limitations to new Nanostructured Thin Film catalyst activity to improve Performance and durability of fuel cells

MERCK
Pfizer

Drug Discovery

Developed a new cryogenic electron tomography (cryo-EM) technique to probe new mechanisms such as the transfer of cholesterol ester proteins for pharmaceuticals development

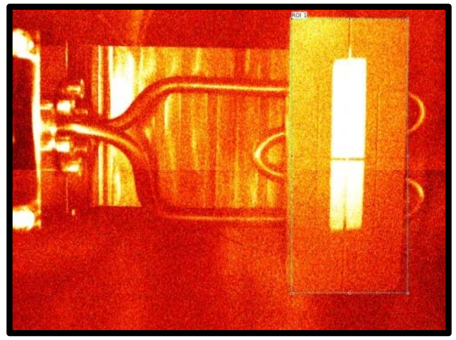


National Synchrotron Light Source-II

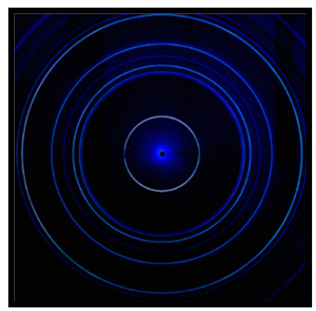
Successfully completed ahead of schedule and within budget

- The project has delivered:
  - A highly optimized electron storage ring with exceptional x-ray brightness and beam stability
  - Six advanced instruments, optics and detectors that capitalize on these capabilities
- Design goals:
  - 1 nm spatial resolution
  - 0.1 meV energy resolution
  - Single atom sensitivity
- First light on October 23, 2014
- All project scope and Key Performance Parameters completed – Dec 2014
- Office of Project Assessment Review Feb. 10-11, 2015, recommending CD-4 approval

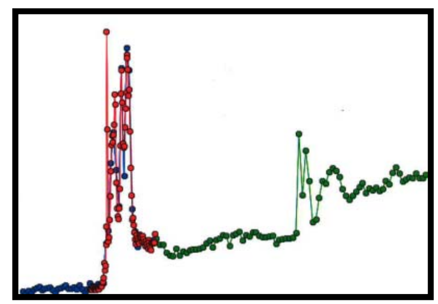
✓ Aug 2005 CD-0, Approve Mission Need
✓ Jul 2007 CD-1, Approve Alternative Selection & Cost Range
✓ Jan 2008 CD-2, Approve Performance Baseline
✓ Jan 2009 CD-3, Approve Start of Construction
✓ Dec 2014 Project Early Completion
✓ Feb 2015 S-1 Dedication of NSLS-II
✓ Mar 2015 CD-4, Approve Start of Operations



NSLS-II First Light at CSX Beamline Oct 23, 2014



First Diffraction Data

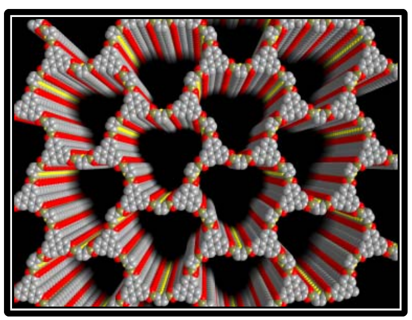


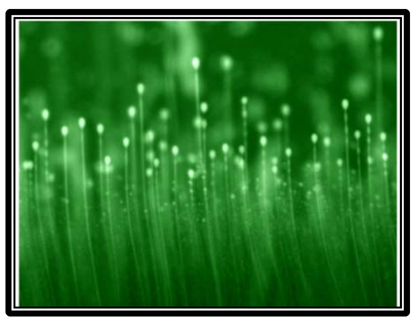
First Spectroscopy Scan

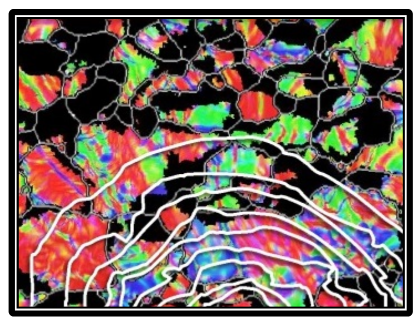
FY 2016 BES Budget Request

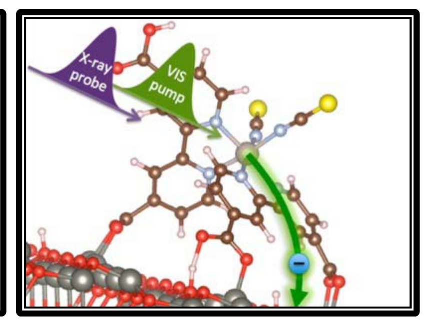
Understanding, predicting, and controlling matter and energy at the electronic, atomic, and molecular levels

- Increased funding for additional **Energy Frontier Research Centers** (EFRCs) (Δ = +$10,000K)
- Increased funding for **computational materials sciences** research to expand technical breadth of code development for design of functional materials (Δ = +$4,000K)
- New funding for **mid-scale instrumentation** for ultrafast electron scattering (Δ = +$5,000K)
- **Energy Innovation Hubs**:
  - Joint Center for Energy Storage Research (JCESR) will be in its 4^{th} year. (FY 15 = $24,175K; FY 2016 = $24,137K)
  - Joint Center for Artificial Photosynthesis (JCAP) is under review for renewal starting in September 2015. (FY 2015 = $15,000K; FY 2016 = $15,000K)
- **National Synchrotron Light Source-II** (NSLS-II) begins its 1^{st} full year of operations.
- **Linac Coherent Light Source-II (LCLS-II)** construction continues.
- BES **user facilities** operate at near optimum levels (~99% of optimal).
- Two **major items of equipment**: NSLS-II Experimental Tools (NEXT) and Advanced Photon Source Upgrade (APS-U) are underway.

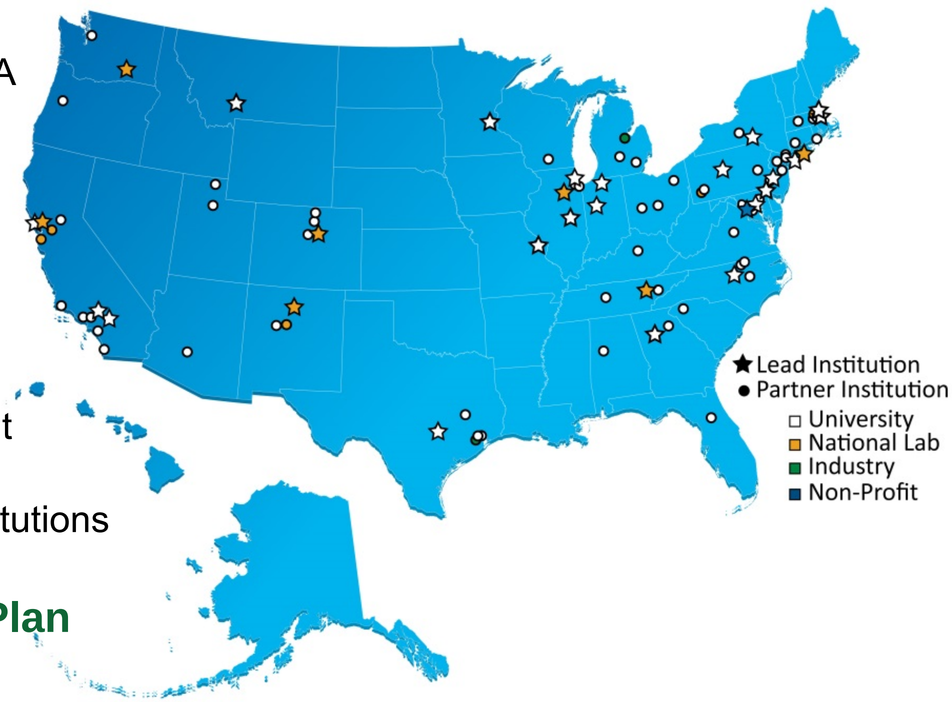








Energy Frontier Research Centers, 2009 - present



FY 2009 46 EFRCs were launched

- $777M for 5 years, $100M/year base + $277M ARRA

FY 2014 Recompetition Results

- $100M/year base
- 32 EFRCs in 32 States + Washington D.C.
  (22 renewals+ 10 new)
- Each $2-4M/yr for up to 4 years
- Led by 23 Universities, 8 DOE Labs, and 1 non-profit
- ~525 senior investigators and ~900 students, postdoctoral fellows, and technical staff at ~100 institutions

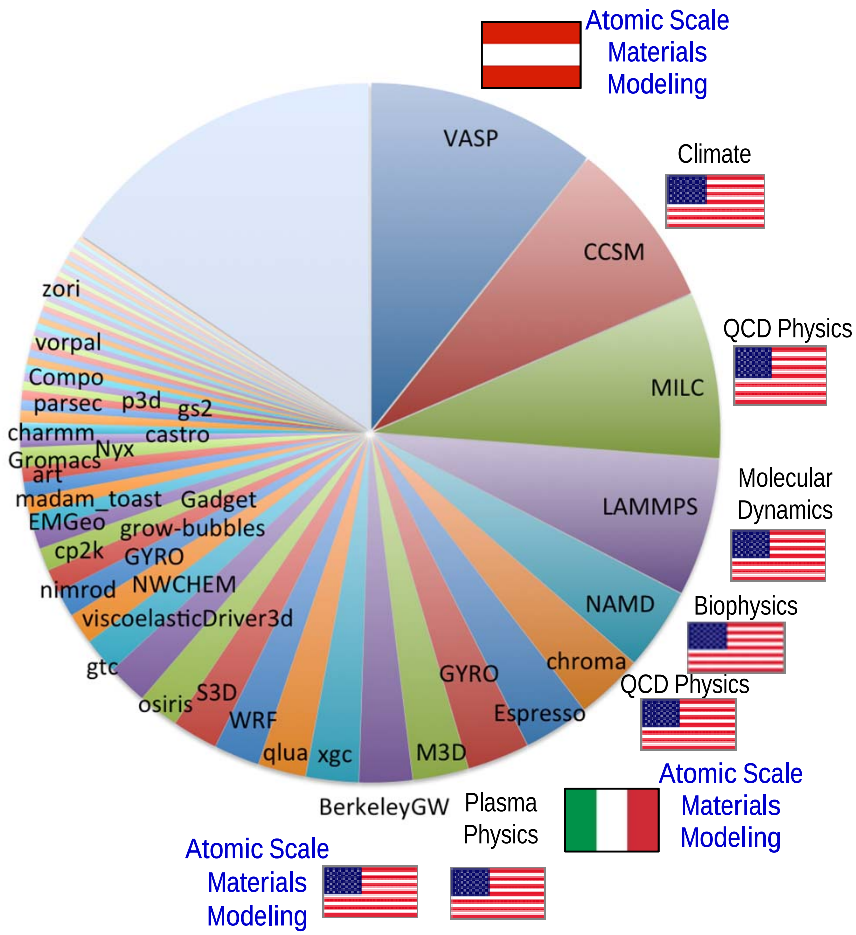
FY 2015 – FY 2016 Review and Management Plan

- Management review of new centers in FY 2015.
- Full mid-term progress review for all centers in FY 2016, with funding for final two years contingent upon review outcome.

FY 2016 Funding and New Solicitation

- Funding for EFRCs increases $10,000K (FY 2015 = $100,000K; FY 2016 = $110,000K).
- Call for new EFRC proposals with topical areas that complement current portfolio and that are informed by new community workshops.
- The EFRC program will transition to a biennial solicitation cycle starting in FY 2016.

Increase for Computational Materials Sciences



2013 Top Application Codes at NERSC

Funding

- FY 2015 included $8M for new awards. FOA announced in January 2015 for proposals for 4-year research projects to be funded at $2-4M per year.
- FY 2016 Request of $12M will continue support for the 2015 awards and will fund additional awards to broaden the technical scope of the research.

Why computational materials sciences? The U.S. trails competitors in computational codes for materials discovery and engineering

- At NERSC, the most used code is VASP, an commercial Austrian atomic scale materials modeling code requiring purchase of license.
- (Quantum) Espresso, a popular materials modeling code, was developed by Italy.
- Top codes for other fields used at NERSC were developed in the U.S. and are all free, community codes.

Basic and Applied Research Coordination

- **Many activities facilitate cooperation and coordination between BES and the technology programs**
  - Joint efforts in strategic planning (e.g., BRN workshops, BES participation in ARPA-E and FCT workshops)
  - Solicitation development
  - Reciprocal staff participation in proposal review activities
  - Joint program contractors meetings
  - Joint SBIR topics
  - Participation by BES researchers at the Annual Merit Review
  - "Tech Teams" formed across DOE

- **Co-funding and co-siting of research by BES and DOE technology programs at DOE labs or universities, has proven to be a viable approach to facilitate close integration of basic and applied research through sharing of resources, expertise, and knowledge of research breakthroughs and program needs.**

Continuum of Research, Development, and Deployment

Discovery Research | Use-Inspired Basic Research | Applied Research | Technology Maturation & Deployment

Office of Science | ARPA-E* | Applied Programs

Goal: new knowledge / understanding
Focus: phenomena
Metric: knowledge generation

Goal: practical targets
Focus: performance
Metric: milestone achievement

- Basic research to address fundamental limitations of current theories and descriptions of matter in the energy range important to everyday life – typically energies up to those required to break chemical bonds.

- Basic research for fundamental new understanding on materials or systems that may revolutionize or transform today's energy technologies

- Basic research for fundamental new understanding, usually with the goal of addressing scientific showstoppers on real-world applications in the energy technologies

- Proof of new, higher-risk concepts
- Prototyping of new technology concepts
- Explore feasibility of scale-up of demonstrated technology concepts in a "quick-hit" fashion.

- Research with the goal of meeting *technical milestones*, with emphasis on the development, performance, cost reduction, and durability of materials and components or on efficient processes

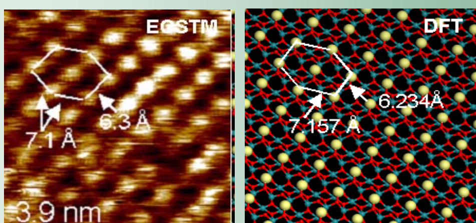
- Scale-up research
- Small-scale and at-scale demonstration
- Cost reduction
- Manufacturing R&D
- Deployment support, leading to market adoption
- High cost-sharing with industry partners

* ARPA-E: targets technology gaps, high-risk concepts, aggressive delivery times

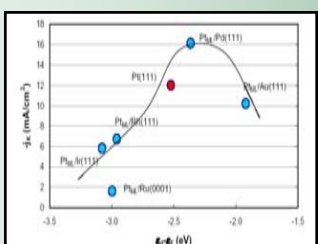
Advanced Fuel Cell Electrocatalysts

BES
Basic Science

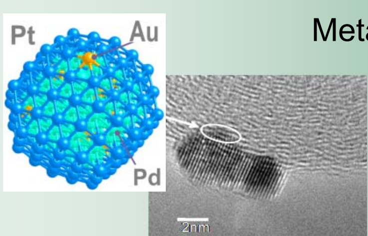
Principles and methods for monolayer electrocatalysis.



In-situ electrochemical studies of structure and catalytic activity of single atomic layers



Discover and develop high activity monolayer platinum catalysts.

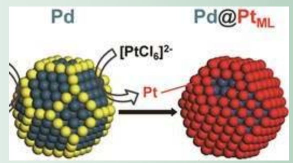


Metal alloys to improve durability

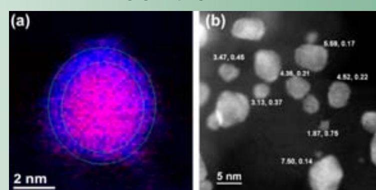
Core-shell electrocatalysts
>100 publications 2001-14
>8000 citations

EERE Fuel Cell Office
Applied Research

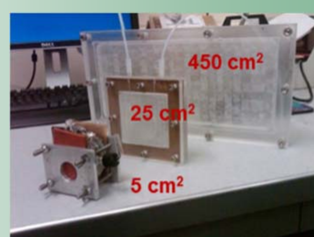
Core-shell electrocatalysts developed for high activity and durability with ultralow Pt mass.



Developed syntheses for nanoscale core-shell catalysts with monolayer control.



Enhanced Pt-mass weighted activity 10x. Scale-up synthesis led to membrane electrode assemblies with good performance.



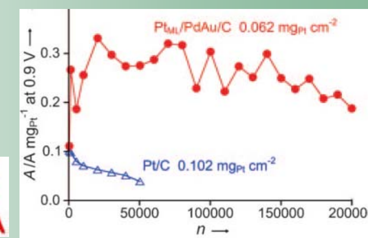
R&D 100 Award

Industrial Collaboration
Toward Deployment

Performance and durability in subsystem membrane electrode assemblies, licensing, manufacture methods

Excellent fuel cell durability 200K cycles with Toyota

TOYOTA

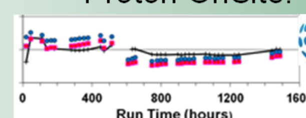


Licensed to NECC, manufacturing scale-up.

N.E. CHEMCAT
Lead The Catalyst Innovations

Excellent electrolyzer performance, >10x reduced Pt mass with Proton OnSite.

PROTON ON SITE



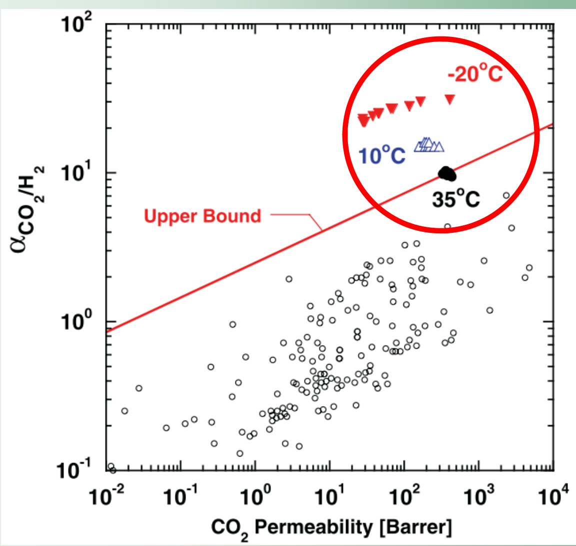
High performance, low Pt electrocatalysts ready for applications in fuel cell vehicles and hydrogen generation.

BROOKHAVEN
NATIONAL LABORATORY

High Performance H_2 Separation Membranes

BES Basic Science

Discovered new polymers with high CO_2 permeability & high CO_2/H_2 selectivity



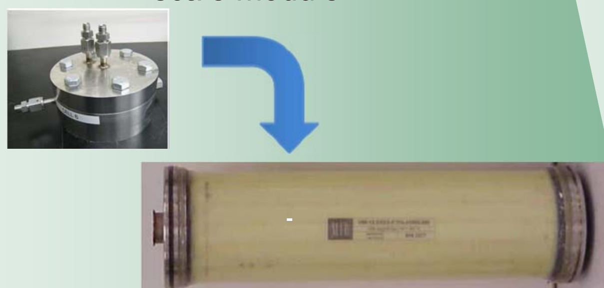
Materials promising for syngas purification, carbon capture, and natural gas separation

Lin, Van Wagner, Freeman, Toy, Gupta. *Science 311, 639 (2006).*

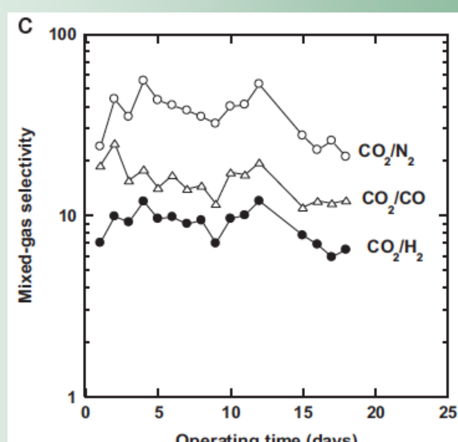
FE Sponsored Applied R&D

Materials manufactured into membrane modules and properties validated on syngas in laboratory and at NCCC

Scaleup from lab samples to commercial scale module



Validation of membrane module separation properties at NCCC



Lin, et al., *J. Membrane Sci. 457, 149 (2014).*

Manufacturing/ Commercialization

Commercial scale membrane modules and systems engineered & manufactured in the USA

227 kg/h syngas membrane unit

Commercial sales of CO_2/H_2 separation systems and H_2S removal from natural gas.

20 ton/day CO_2 capture system installed and operated at NCCC.

Nanoframes with 3D Electrocatalytic Surfaces

Scientific Achievement

Nanoframe architecture with controlled surface structure, compositional profile and surfaces with three dimensional molecular accessibility

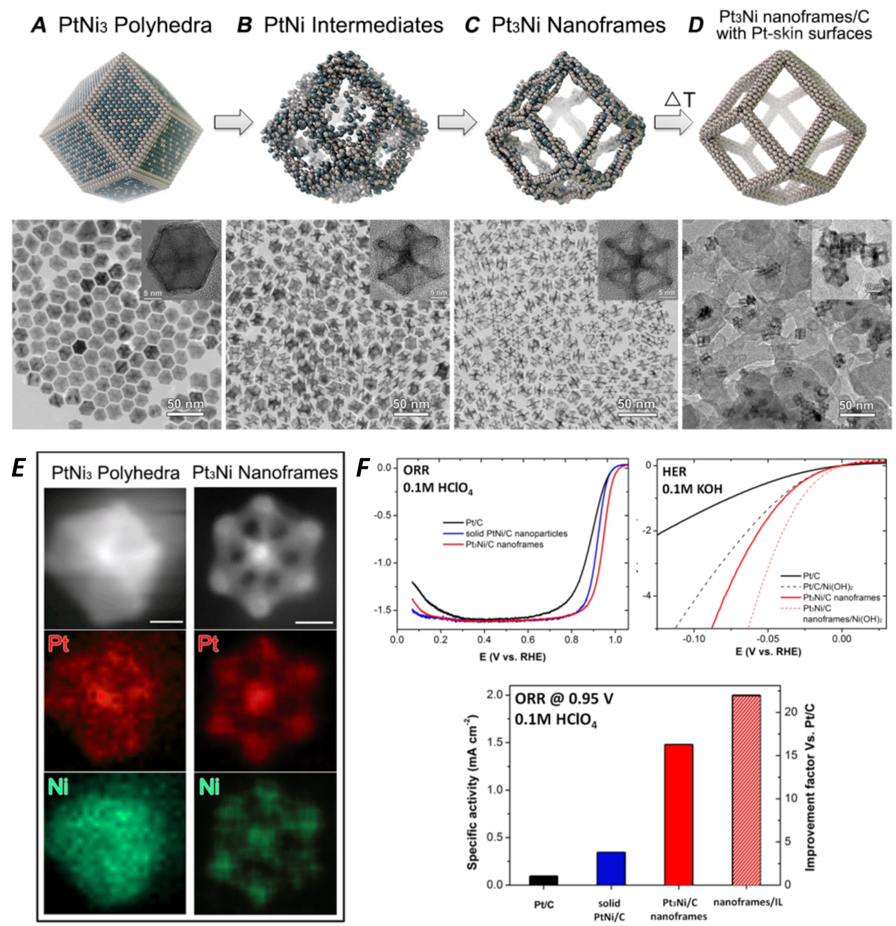
Significance and Impact

Superior electrocatalytic properties of highly crystalline multimetallic nanoscale materials

Research Details

- Structural evolution from $PtNi_3$ solid bimetallic polyhedra to Pt_3Ni hollow nanoframes
- Surface is tuned to form desired Pt-Skin structure
- Superior catalytic activities for the oxygen reduction and hydrogen evolution reactions have been achieved for highly crystalline multimetallic nanoframes
- Collaborative effort between Lawrence Berkeley National Laboratory and Argonne National Laboratory

NOW SUPPORTED BY THE FCTO



Multimetallic nanoframes with 3D surfaces:
Structural evolution of nanoparticles from: **(A)** polyhedra, **(B)** intermediates, **(C)** nanoframes and **(D)** nanoframes with multilayered Pt-Skin structure; **(E)** elemental mapping and **(F)** superior electrochemical activities for ORR and HER

Work was performed at Lawrence Berkeley and Argonne National Laboratories
Science ***343***(2014) 1339-1343

Proton Transport Mechanism and the Effect of Polymer Morphology in Proton Exchange Membranes

Scientific Achievement

A large increase in proton conductance is predicted if hydrated excess protons can move into the water-rich regions from being trapped near the polymer sulfonate side chains.

Significance and Impact

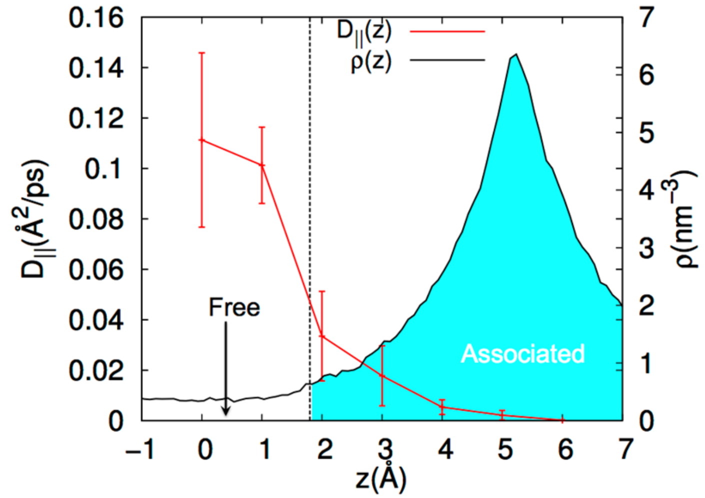
Different polymer morphologies were also found to exhibit different proton transport behavior as a function of hydration at the mesoscale.[1]

Research Involved

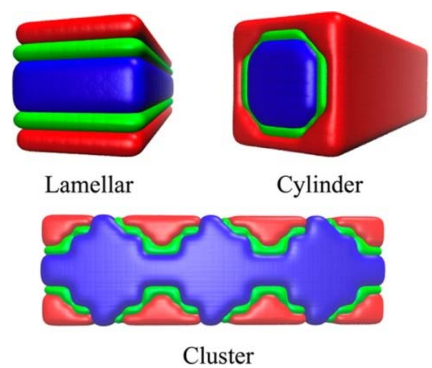
- Using novel, large scale reactive MD simulations[2] it was quantitatively shown that hydrated excess proton diffusion at the hydrophilic pore center can be much faster than near the sulfonate side chains (see figure at upper right).
- However, the hydrated protons reside preferentially near the sulfonate side chains due to electrostatic interactions.
- Mesoscopic simulations[1] for the polymer morphologies (lower right) were parameterized using the MD simulations.
- Due to its tortuosity, the proton conductivity of the cluster morphology was found to be significantly lower than for lamellar and cylinder morphologies. A morphological transition upon hydration was also predicted (far right panel).

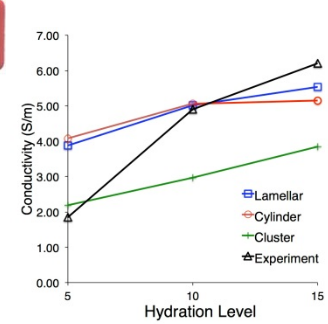
(1) Liu, S.; Savage, J.; **Voth, G. A.**, *J. Phys. Chem. C* **2015,** *119*, 1753-1762

(2) Savage, J.; Tse, Y.-L. S; **Voth, G. A.**, J. Phys. Chem. C **2015**, *118*, 17436–17445



The **red line** is the hydrated proton diffusion constant at different positions from the center of the lamellar channel (z = 0 Å) to the region of sulfonate groups on the polymer interface (z = 6 Å). The **excess proton probability** is also shown.

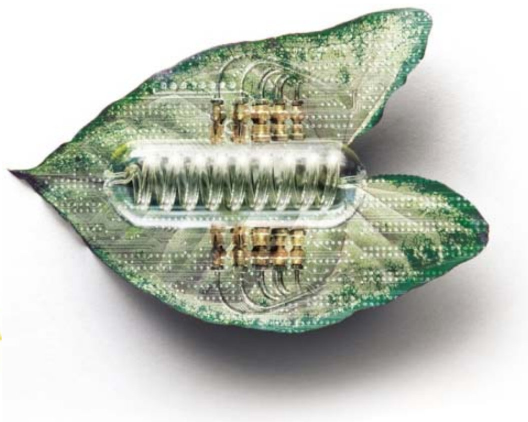




Leaky TiO_2-stabilized Photoanodes for Efficient Production of Hydrogen and Other Solar Fuels

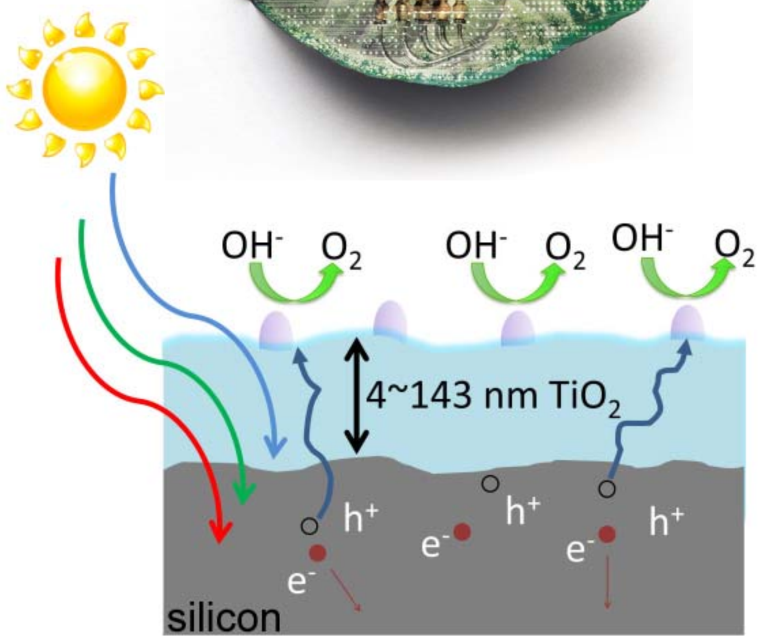
Scientific Achievement

A new method was devised that protects common semiconductors from corrosion in basic aqueous solutions while still maintaining excellent electrical charge conduction



Significance and Impact

Efficient light-absorbing semiconductors that corrode when unprotected can now be used as photoanodes in a solar fuels generator for hydrogen production



Photoanode stabilized against corrosion in an aqueous KOH electrolyte by a thick, electronically defective layer of unannealed TiO_2 produced by atomic layer deposition.

Hu, S., *et. al*, *Science*, 344, 1005-1009 (2014). DOI: 10.1126/science.1251428

Research Details

- Scientists are trying to develop solar-driven generators to split water, yielding hydrogen and other fuels.
- Common semiconductors that are efficient light absorbers often corrode in basic aqueous solutions used for the device.
- Atomic layer deposition was used to coat semiconductors with an electronically defective ~100 nm layer of unannealed TiO_2, protecting the conductor from corrosion
- In conjunction with islands of nickel oxide electrocatalysts, protected silicon seminconductors continuously and stably oxidized water for over 100 hours at photocurrents of >30 mA cm^{-2} under 1-sun illumination

Light-Driven Hydrogen Production via Photosystem I and a Nickel Catalyst

Scientific Achievement

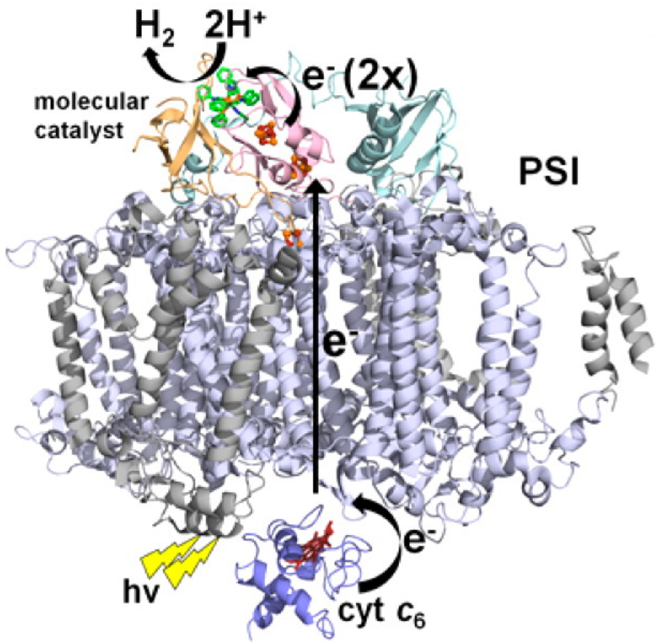
First example of hydrogen formation via a biohybrid consisting of a synthetic molecular nickel (Ni) catalyst and cyanobacterial Photosystem I (PSI) reaction center in completely aqueous conditions and at near-neutral pH.

Significance and Impact

This strategy could enable photocatalytic hydrogen production using earth-abundant materials by linking synthetic designs with natural reaction center photochemistry.

Research Details

- A new strategy was developed using protein-directed delivery of a Ni molecular catalyst to the reducing side of PSI for light-driven catalysis
- This self-assembled PSI/Ni hybrid generated hydrogen at a rate 2 orders of magnitude greater than that reported for photosensitizer/Ni systems.
- Photocatalysis was observed at pH 6.3 in completely aqueous conditions.



Photocatalytic model of H_2 production from a PSI-Ni hybrid complex via the transfer of two successive photogenerated electrons from PSI to a bound Ni molecular catalyst. The exact position of the Ni catalyst on the acceptor end of PSI is not known

Silver *et. al*, *J. Am. Chem. Soc.*, **2013**, *135* (36), pp 13246–13249 **DOI:** 10.1021/ja405277g

Computational Screening of Metal-Organic Frameworks for Hydrogen Storage

Scientific Achievement

Structure-property relationships and top materials were predicted for hydrogen storage in metal-organic frameworks (MOFs) by computational screening of >18,000 MOF structures.

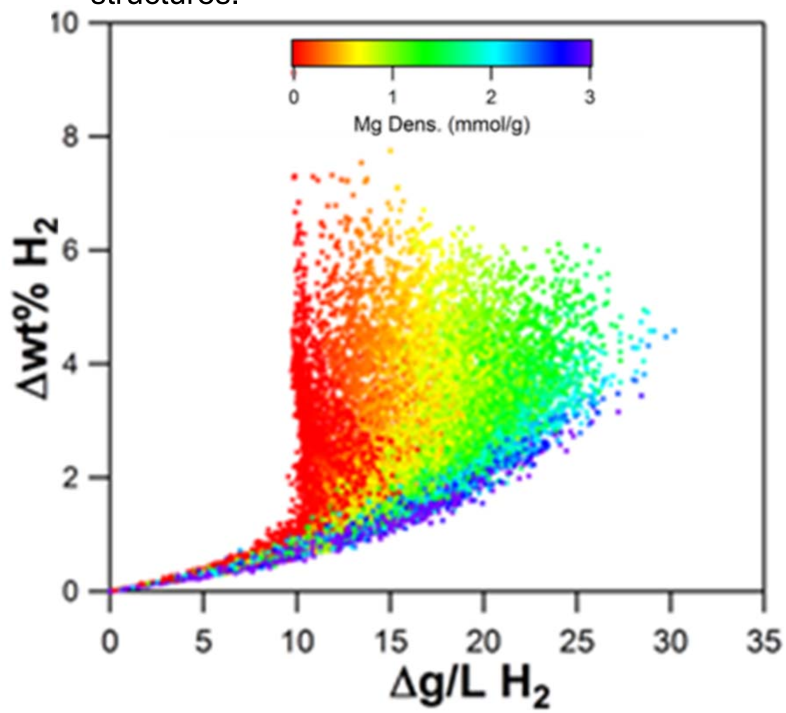
Significance and Impact

Tradeoffs are revealed between gravimetric storage and volumetric storage. Results show that it may be difficult to meet both targets simultaneously.

Research Details

- A library of MOFs having a diverse range of pore sizes, surface areas, etc. were generated computationally.
- Magnesium alkoxide functional groups were added to the MOFs. Previous work had shown that Mg alkoxides provide near-optimum enthalpies of adsorption – high enough to adsorb hydrogen at high pressure, but low enough to release the hydrogen for utilization.
- Monte Carlo simulations were used to predict deliverable hydrogen capacity.

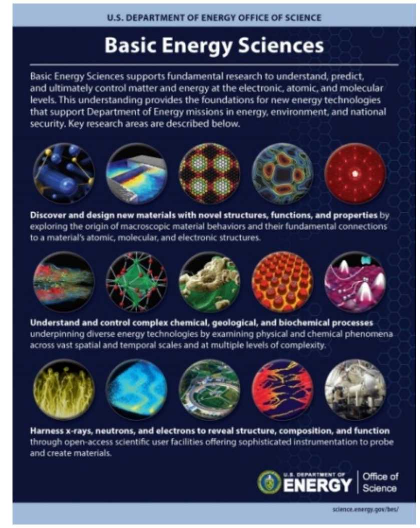
Gravimetric vs. volumetric hydrogen storage are plotted for deliverable capacities at 243 K for a filling pressure of 100 bar and a delivery pressure of 2 bar. The colors represent the density of Mg alkoxide functional groups in the structures.



Y.J. Colón, D. Fairen-Jimenez, C.E. Wilmer, R.Q. Snurr, "High-throughput screening of porous crystalline materials for hydrogen storage capacity near room temperature," J. Phys. Chem. C 118, 5383−5389 (2014).

BES Communications

- **BES Brochure**
  - 11”x17” brochure describing BES-supported research, tools, and facilities
  - Examples illustrate BES investments in:
    - research ranging from discovery science to science for energy technologies, and
    - tools including laboratory equipment, theory and experiment, and large user facilities.



- **BES Research Summaries**
  - Report describing over 1200 BES-supported research projects in FY 2014
  - Each entry includes the title, senior investigators, number of students and postdocs, institutions, funding level, program scope, and FY 2014 highlights.