U.S. DEPARTMENT OF ENERGY | Office of Science

Basic Energy Sciences Update

2015 DOE HYDROGEN and FUEL CELLS PROGRAM and VEHICLE TECHNOLOGIES OFFICE ANNUAL MERIT REVIEW and PEER EVALUATION MEETING

June 8, 2015

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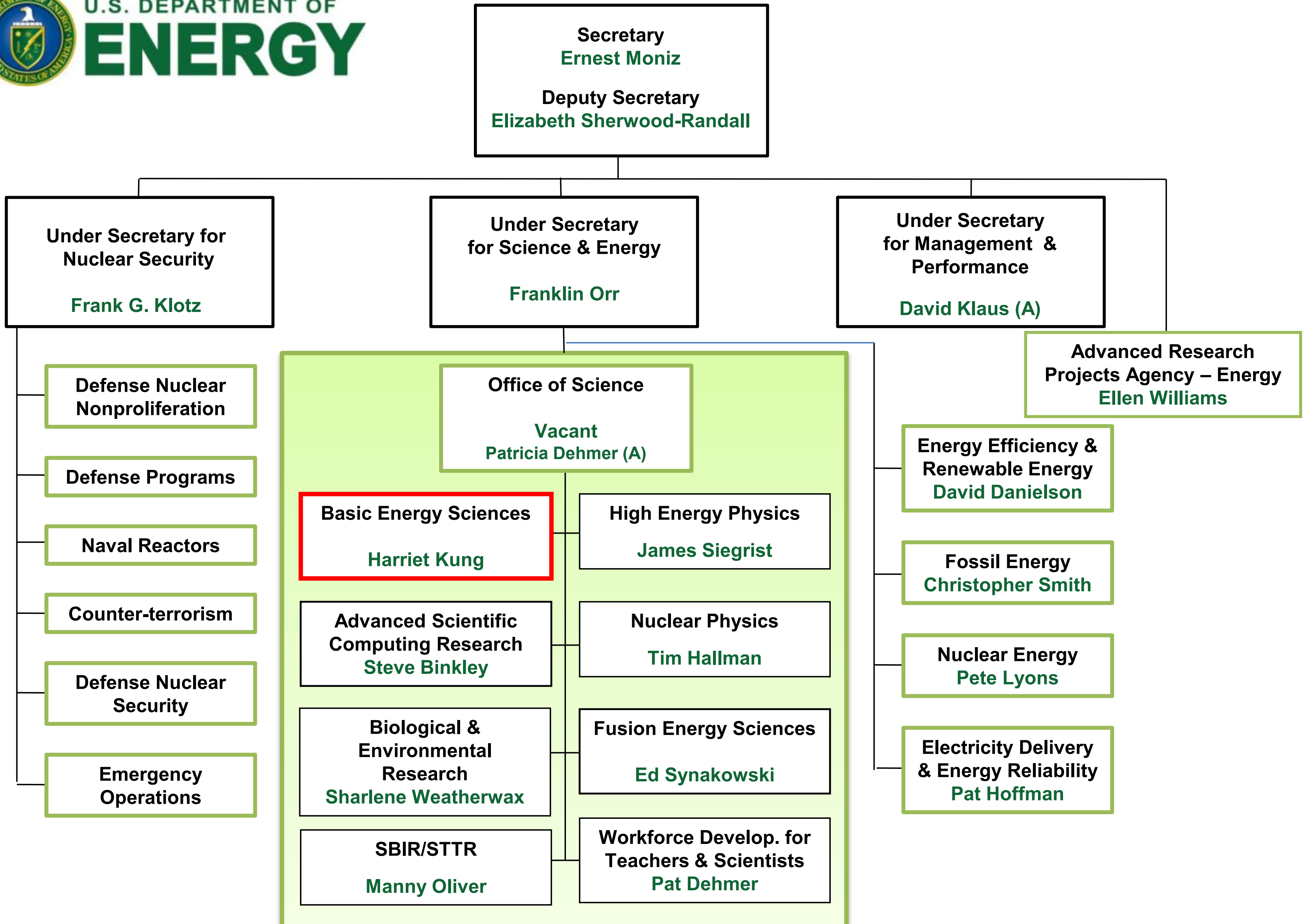
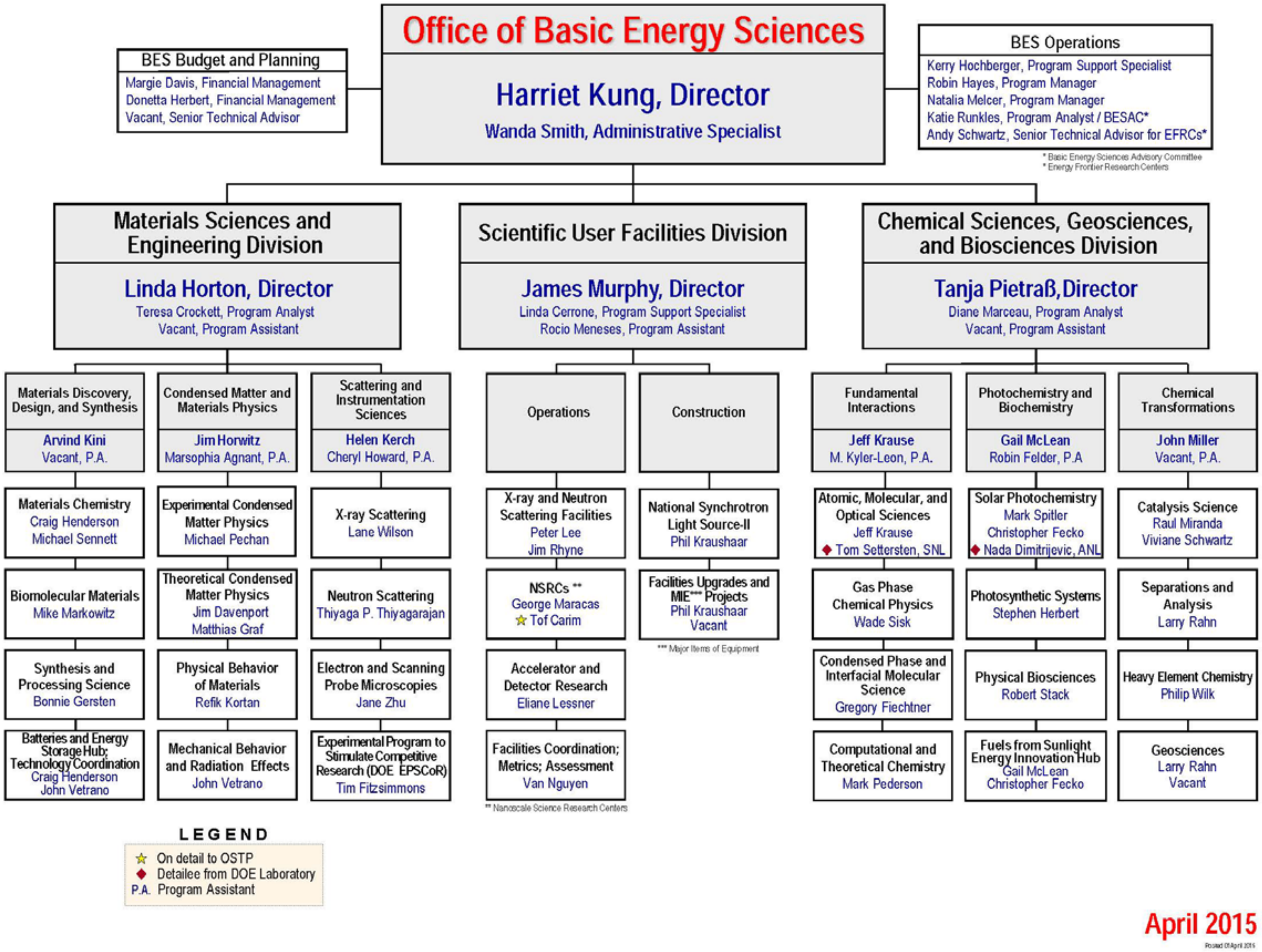
Office of Science/Basic Energy Sciences
U.S. Department of Energy

U.S. DEPARTMENT OF ENERGY



Organization – Basic Energy Sciences



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 Biosciences—exploring the fundamental aspects of chemical reactivity and energy transduction over wide ranges of scale and complexity and their applications to energy technologies

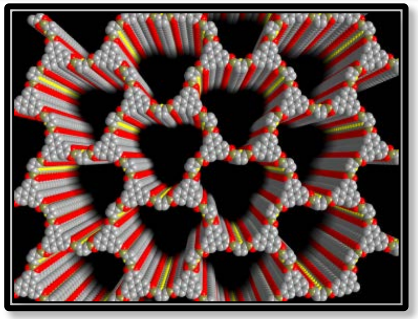
Supporting:

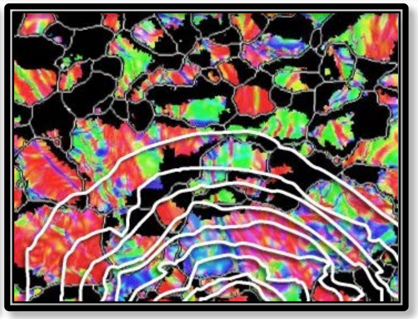
- 32 Energy Frontier Research Centers
- Fuels from Sunlight & Batteries and Energy Storage Hubs
- The largest collection of facilities for electron, x-ray, and neutron scattering in the world

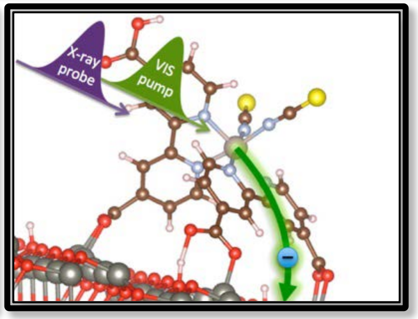
The Scientific Challenges:

- 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





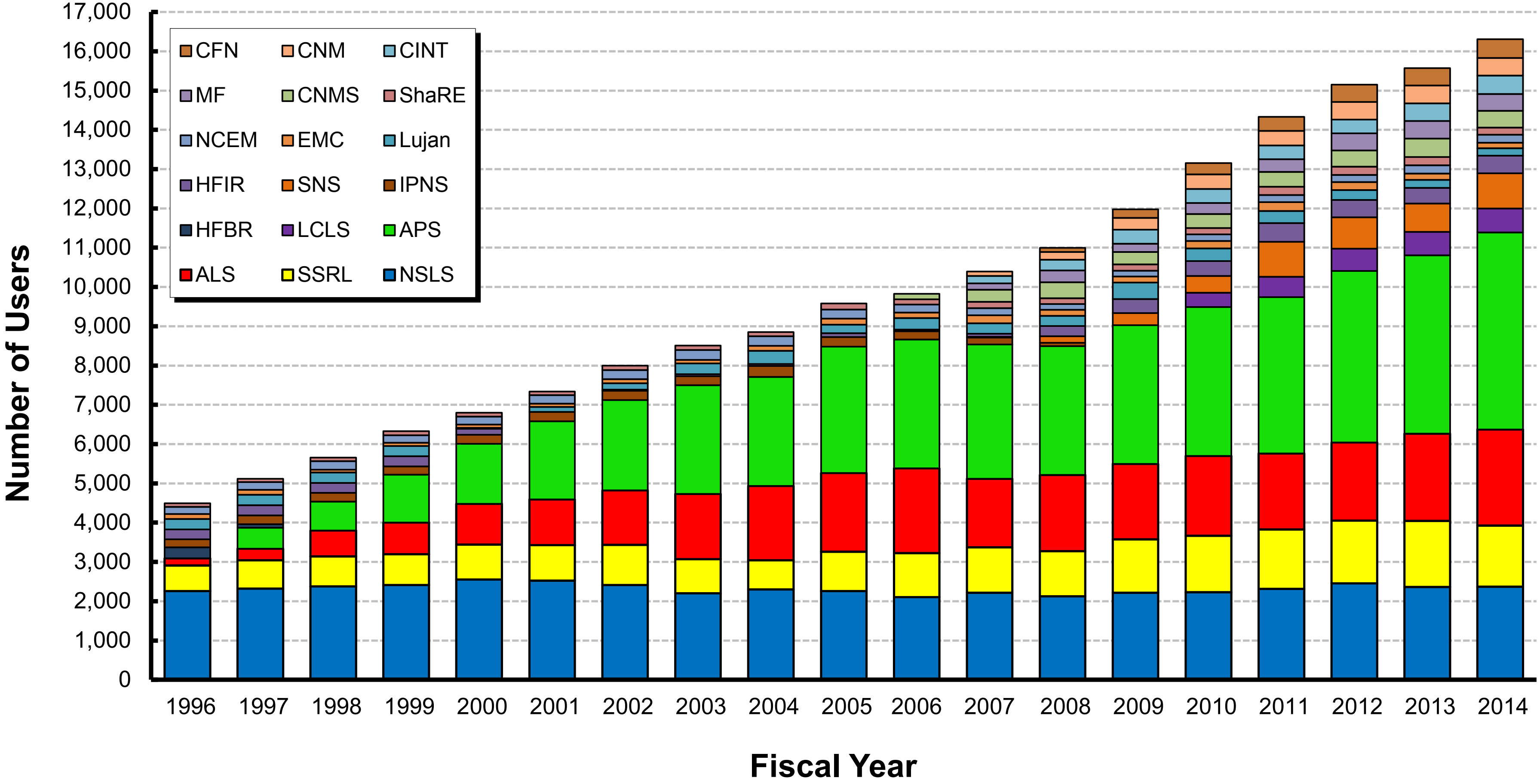


BES User Facilities
Serving over 16,000 Users in FY 2014

Unique research facilities *and* scientific expertise for ultra high-resolution characterization, synthesis, fabrication, theory and modeling of advanced materials

- **Light sources**
  - *Stanford Synchrotron Radiation Laboratory (SLAC)*
  - *National Synchrotron Light Source- II under construction (BNL)*
  - *Advanced Light Source (LBNL)*
  - *Advanced Photon Source (ANL)*
  - *Linac Coherent Light Source (SLAC)*
- **Neutron sources**
  - *Manuel Lujan, Jr. Neutron Scattering Center (LANL)*
  - *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)*
- **Electron-Beam Microcharacterization Centers (merged with the NSRCs starting in FY 2015)**
  - *Electron Microscopy Center for Materials Research (ANL)*
  - *National Center for Electron Microscopy (LBNL)*
  - *Shared Research Equipment Program (ORNL)*

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.

BES Nanoscale Science Research Centers—
Completed in 2006 – 2008, Serving >2000 users/Yr

Center for Functional Nanomaterials (Brookhaven National Laboratory, NY)

Molecular Foundry (Lawrence Berkeley National Laboratory, CA)

Center for Nanoscale Materials (Argonne National Laboratory, IL)

Center for Nanophase Materials Sciences (Oak Ridge National Laboratory, TN)

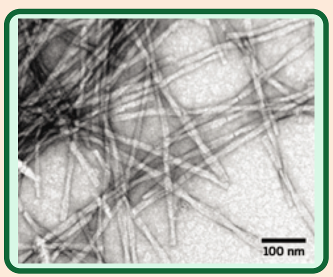
Center for Integrated Nanotechnologies (Sandia & Los Alamos National Labs, NM)

Industry Use of Nanoscale Science Research Centers

NOVARTIS

Disease Therapeutics

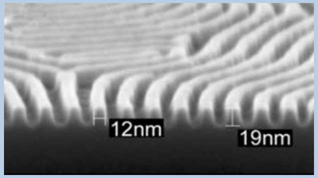
Groundbreaking nanoscience highly sensitive technique for detecting misfolded proteins could help pinpoint Alzheimer's in its early stages and enable researchers to discover new disease therapies.



HGST
a Western Digital company

Ultradense Memories

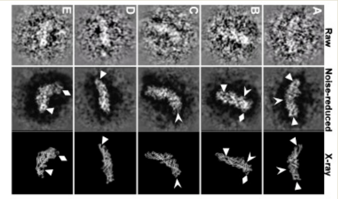
Expertise in polymer nanostructure self-assembly and electron microscopy can be applied to Terabit/cm^2 scale magnetic memories for computing and imaging



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



3M

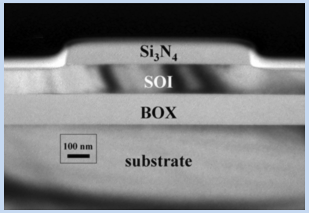
High Performance Fuel Cells

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

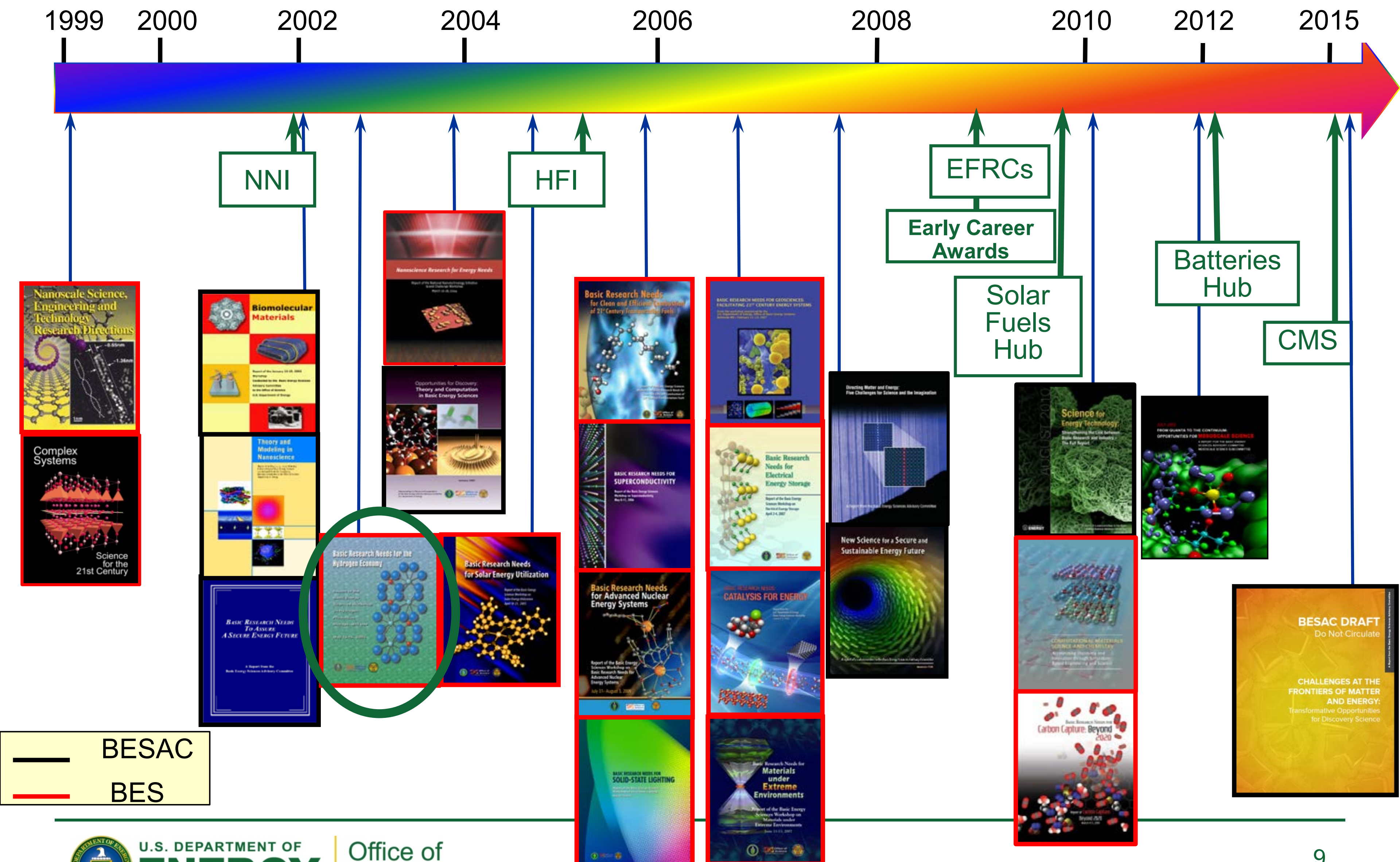
IBM

Advanced Microprocessors

Unique NSRC hard x-ray Nanoprobe enables nondestructive measure of in-situ strain distributions in silicon-on-insulator (SOI)-based CMOS for sub 75 nm microprocessor technology.



BES Strategic Planning and Program Development



http://science.energy.gov/bes/news-and-resources/reports/

BES Strategic Planning and Program Development

Basic Research R&D Plan: BES Hydrogen Workshop Report

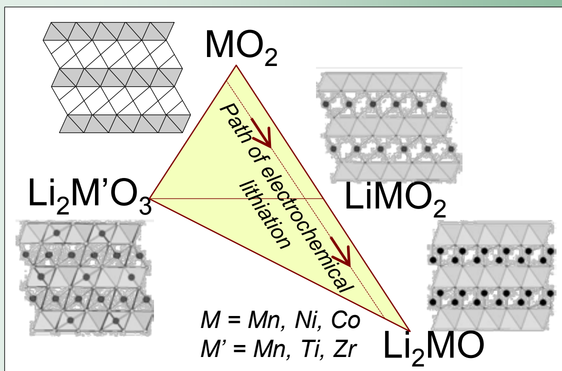
May 13-15, 2003

"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**."

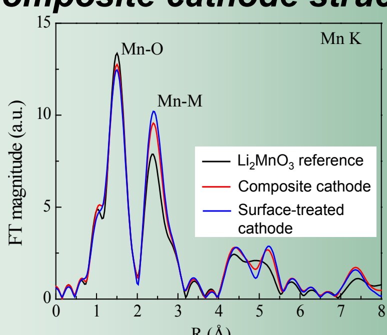
High-Energy Lithium Batteries: From Fundamental Research to Cars on the Road

BES Basic Science

Discovered new nanostructured composite cathode materials and interfaces



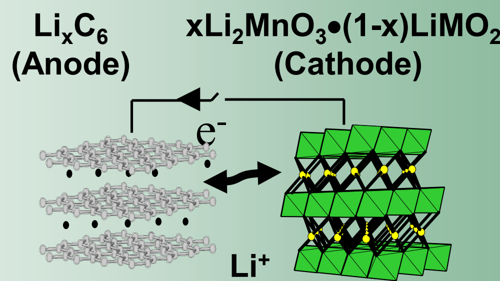
Used the Advanced Photon Source to characterize and understand composite cathode structures



Fourier-transformed X-ray absorption data of a composite cathode structure

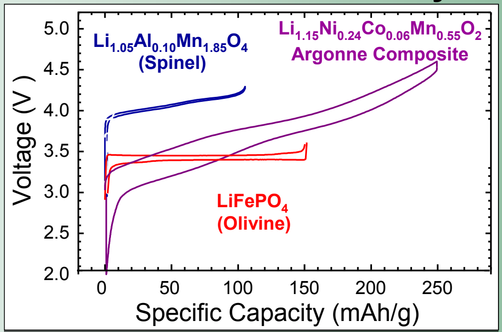
EERE Applied R&D

Used advanced composite cathode materials to create high energy lithium ion cells with improved performance



High energy Li-ion cells…

…with increased cathode capacity, enhanced stability



Manufacturing/ Commercialization

Patents for new cathodes from the basic and applied research are licensed to materials and cell manufacturers and automobile companies

GM

VOLT

BASF The Chemical Company

LG Chem

TODA KOGYO CORP.

Argonne NATIONAL LABORATORY

BES Funding Modalities

Increasing scope and size

- **Core Research (>1,400 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**
  - Fundamental grand challenge and use-inspired research related to topics described in the Basic Research Needs workshop reports
  - 46 centers established in 2009 ($2-5 million/year, 5 years)
  - 32 centers (22 renewal, 10 new) awarded in 2014 ($2-4 million/year, 4 years)

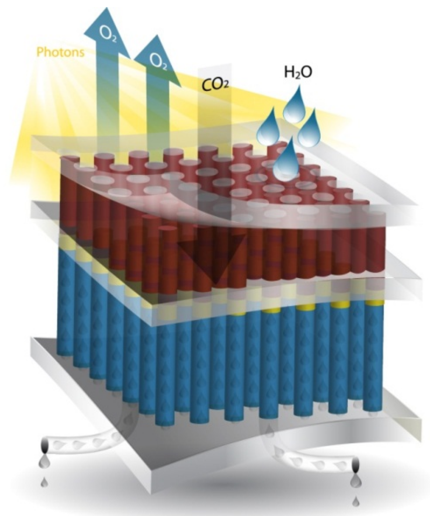
- **Energy Innovation Hubs (2)**
  Research centers, program established in 2010 ($20-25 million/year), engage in basic and applied research, including technology development, on a high-priority topic in energy that is specified in detail in an FOA. Project goals, milestones, and management structure are a significant part of the proposed Hub plan.

BES Research Activities

1. Energy Innovation Hubs

Areas of relevance to AMR:

- Hydrogen generation and storage; membranes
- Energy storage: batteries
- Combustion
- Lightweight materials



Photoelectrochemical Solar-Fuel Generator

Fuels from Sunlight Hub

Joint Center for Artificial Photosynthesis (JCAP)

Overview:

- **Mission:** Develop a solar-fuels generator to produce fuel from the sun 10x more efficiently than crop plants
- Launched in Sept. 2010; DOE announced renewal in April 2015
- Led by Caltech with LBNL as primary partner
- **First Funding Cycle:** Development of prototypes capable of efficiently producing hydrogen via photocatalytic water splitting
- **Second Funding Cycle:** 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

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

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

Bench-top prototype flow battery

Leaky TiO_2-Stabilized Photoanodes for Solar Fuel Production

Scientific Achievement

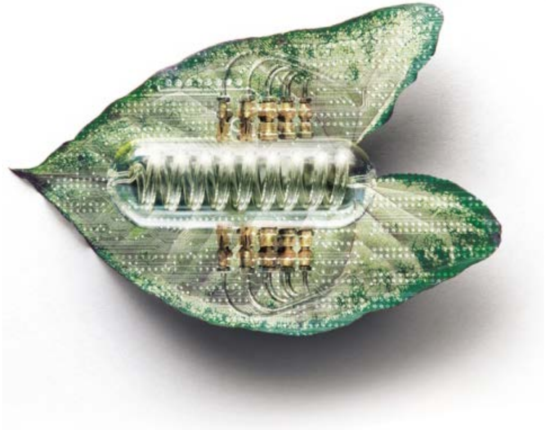
Devised a new method to protect common semiconductors from corrosion in basic aqueous solutions while still maintaining excellent electrical charge conduction to the surface.

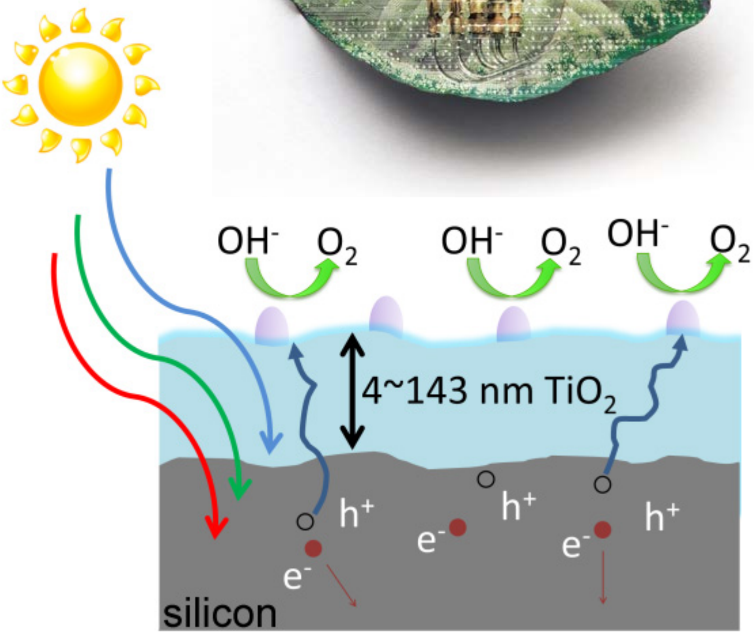
Significance and Impact

Highly light-absorbing semiconductors such as silicon and gallium arsenide corrode when unprotected but can now be incorporated in photoanodes for solar fuel generators.

Research Details

- Semiconductors are protected by an electronically defective layer of ~100 nm thick, unannealed titanium dioxide (TiO_2) using atomic layer deposition
- In conjunction with islands of nickel oxide electrocatalysts, protected silicon can continuously and stably oxidize water for over 100 hours at photocurrents of >30 mA cm^{-2} under 1-sun illumination

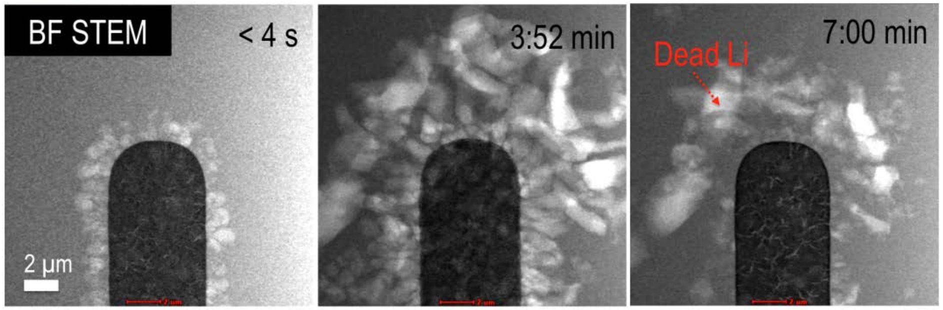




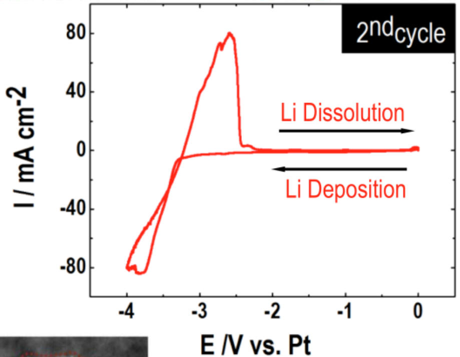
Bottom image: Photoanode stabilized against corrosion in an aqueous KOH electrolyte by a thick, electronically defective layer of unannealed TiO_2 produced by atomic layer deposition.

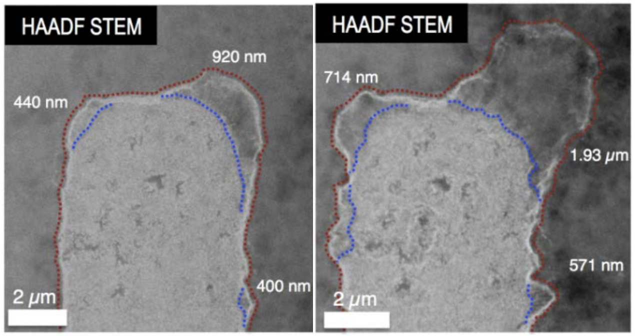
Hu, S., *et. al*, *Science*, 344, 1005-1009 (2014). Top image from *Nature*, 510, 23-24 (2014) News Feature

Direct Observation of SEI and Dendrite Dynamics by *Operando* Electrochemical Scanning Transmission Electron Microscopy



Above: Li deposited on the Pt anode at the beginning (left) , during (middle) and end (right) of the second cycle. Residual “dead Li” can be seen around the anode. *Right:* Simultaneous cyclic voltammetry of the second Li deposition/dissolution cycle.





Left: Evolution of the anode surface roughness (blue line) and dendrite growth beneath the ~200nm thick SEI layer (red line) after extended cycling

Work performed at Pacific Northwest National Laboratory (JCESR partner), Florida State University, UC Davis and Penn State by BL Mehdi, J Qian, E Nasybulin, H Mehta, WA Henderson, W Xu, CM Wang, JE Evans, J Liu, JG Zhang, KT Mueller, ND Browning, C Park, DA Welch, R Faller and KT Mueller, *Nano Letters*, **2015**, DOI: 10.1021/acs.nanolett.5b00175

Scientific Achievement

- Implemented “battery in a STEM” - an *operando* electrochemical stage inside an C_s-corrected scanning transmission electron microscope (STEM)
- Quantified the dynamics of the Solid-Electrolyte Interphase (SEI) layer formation, evolution of anode surface roughness and dendrite nucleation – key features defining the performance and failure modes of next generation Li batteries

Significance and Impact

- First observation of surface reactions and morphology evolution at an anode surface under operating conditions with nanoscale resolution
- Operando stage allows rapid visualization and testing of a wide range of next generation electrode/electrolyte combinations

Research Details

- Mass/thickness contrast uniquely identifies Li from other components in the battery
- Electric field simulation identifies the locations of electrochemical activity
- Pt working electrode in an electrolyte of $LiPF_6$ in propylene carbonate (PC)

BES Research Activities

2. Energy Frontier Research Centers

Areas of relevance to AMR:

- Hydrogen generation and storage; membranes
- Energy storage: batteries
- Combustion
- Lightweight materials

Energy Frontier Research Centers

EFRCs 2009 - 2014

Participants:

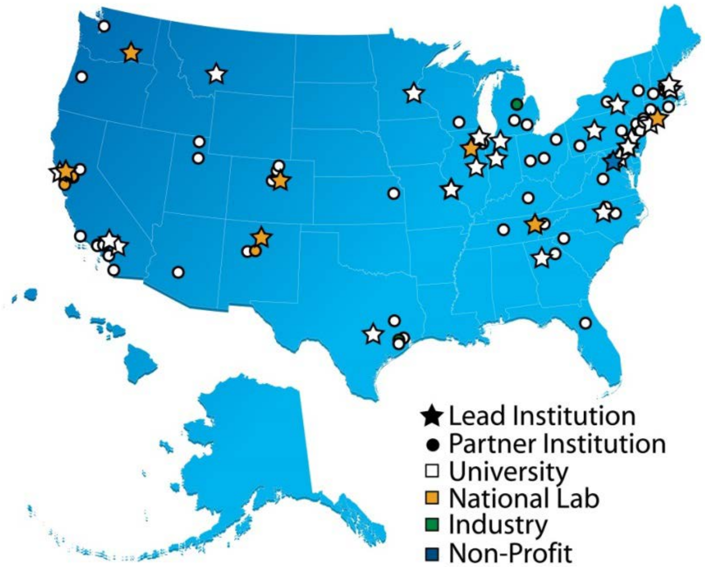
- 46 EFRCs in 35 States + Washington D.C.
- ~850 senior investigators and ~2,000 students, postdoctoral fellows, and technical staff at ~115 institutions
- > 260 scientific advisory board members from 13 countries and > 40 companies

Progress to-date (~5 years funding):

- Nearly 6,000 peer-reviewed papers including >215 publications in *Science* and *Nature*
- 17 PECASE and 15 DOE Early Career Awards
- 37 EFRCs have created over 280 US and 180 foreign patent applications, nearly 100 patent/invention disclosures, and at least 70 licenses
- ~ 70 companies have benefited from EFRC research
- EFRC students and staff now work in: > 300 university faculty and staff positions; > 475 industrial positions; > 200 national labs, government, and non-profit positions

Current EFRCs

- 32 awards of $2-4 million per year
- Lead institutions by type: 23 universities; 8 DOE National Laboratories; 1 nonprofit organization
- Over 100 participating institutions, located in 33 states plus the District of Columbia
- 525 senior investigators and an additional estimated 900 researchers, including postdoctoral associates, graduate students, undergraduate students, and technical staff



Graphene Gateway

Scientific Achievement

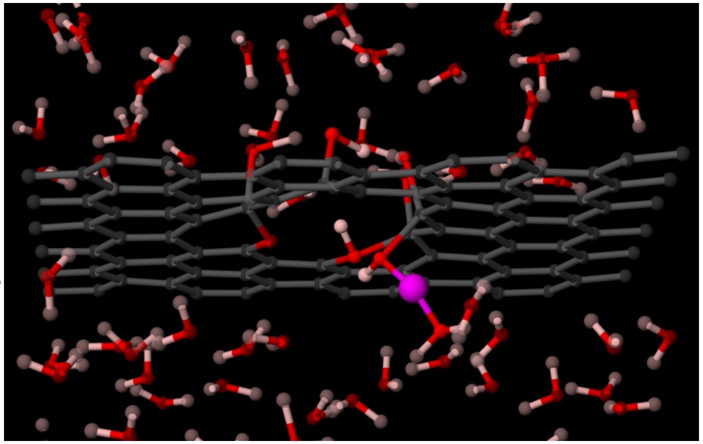
Imaging of atomic scale defects. Computational analysis shows high selectivity for protons.

Significance and Impact

Even hydrogen and helium are too large to pass through the gaps. The high selectivity for proton transport could have significance for designing membranes in fuel cells.

Research Details

- Creation of an atomically thin layer of graphene on fused silica
- Analysis of the graphene using an aberration-corrected scanning transmission electron microscope for direct imaging of individual carbon atoms and “missing” atoms
- Transfer to a silica surface separated by a thin layer of water created a proton trap and allowed for proton transfer detection, using second harmonic generation.
- Substantiation by computational methods.



Computer simulations show a single proton (pink) can cross graphene by passing through the world’s thinnest proton channel. Image courtesy of Franz Geiger, Northwestern University

Fluid Interface Reactions, Structures, and Transport (FIRST)

J. L. Achtyl et al.: Nature Communications 6, 6359, 17 March 2015

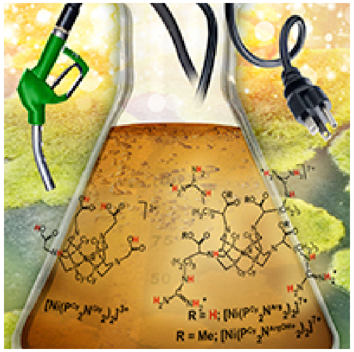
BES Research Activities

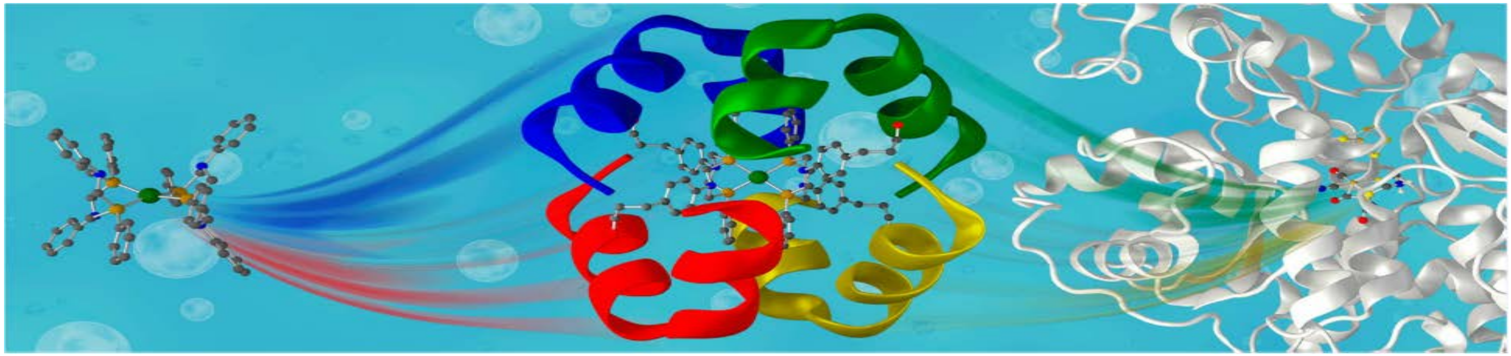
3. Core Research

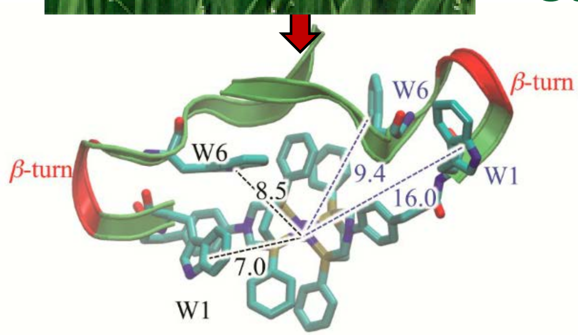
Areas of relevance to AMR:

- Hydrogen generation and storage; membranes
- Energy storage: batteries
- Combustion
- Lightweight materials

Mimicking Biology to Create Fast, Efficient Catalysts







The Science

Researchers have investigated the essential features of the outer coordination sphere of enzymes such as hydrogenase and mimicked those features in artificial catalysts.

The Impact

The altered catalysts have exhibited improved speed by orders of magnitude, along with the ability to function reversibly.

Summary

- The addition of the β-hairpin to the DuBois catalytic core improves the speed of the catalyst, while also providing a platform for developing other features of the outer sphere.
- Added outer sphere features have created the first reversible catalyst that is fast and efficient in both directions. This ability is reminiscent of a catalyst that functions similar to an enzyme.

Nanoframes with 3D Electrocatalytic Surfaces

Scientific Achievement

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

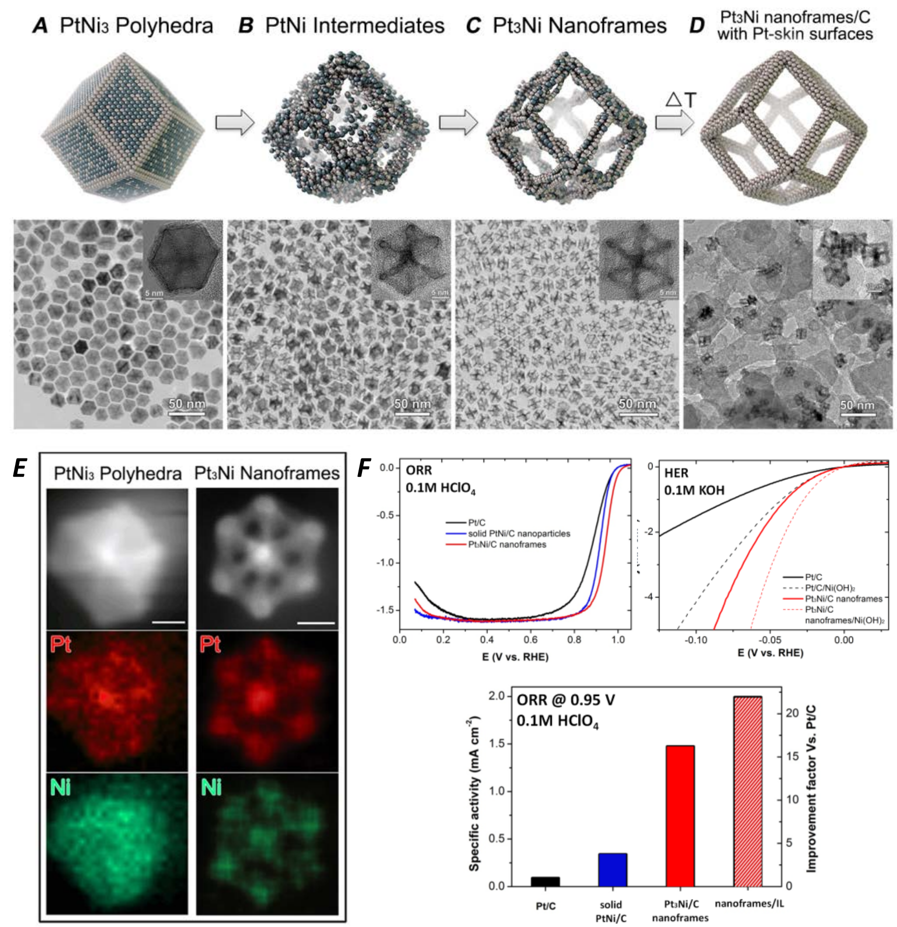
Significance and Impact

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

CONCURRENTLY 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

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.

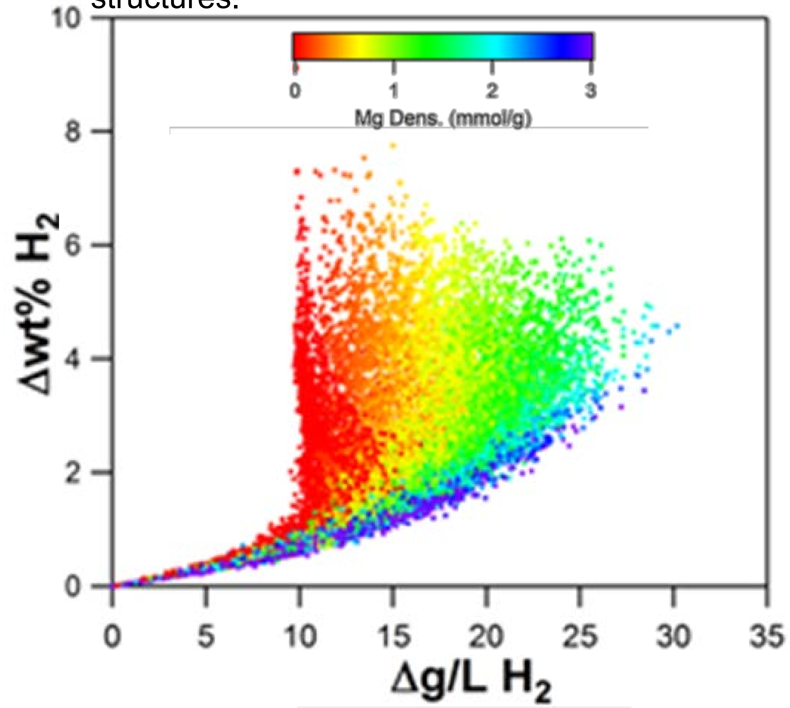
Significance and Impact

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).

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

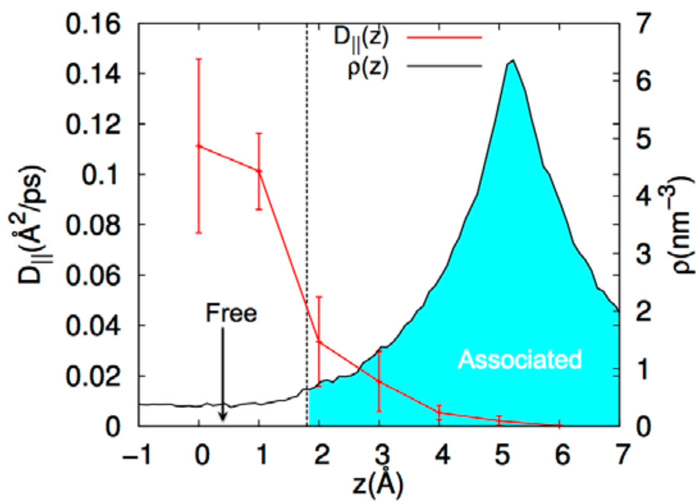
Different polymer morphologies were also found to exhibit different proton transport behavior as a function of hydration at the mesoscale.[1]

Research Involved

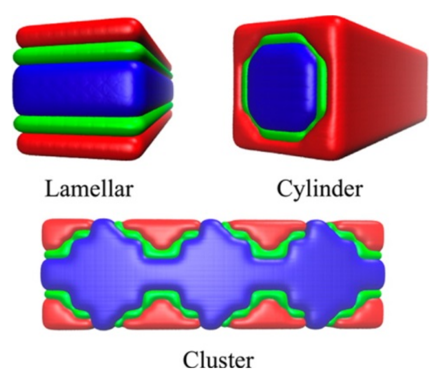
- Using novel, large scale reactive MD simulations[2] it was quantitatively shown that hydrated excess proton diffusion at the hydrophilic pore center can be much faster than near the sulfonate side chains (see figure at upper right).
- However, the hydrated protons reside preferentially near the sulfonate 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).

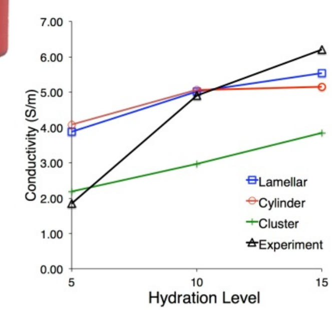
(1) Liu, S.; Savage, J.; **Voth, G. A.**, *J. Phys. Chem. C* **2015**, *119*, 1753-1762

(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.



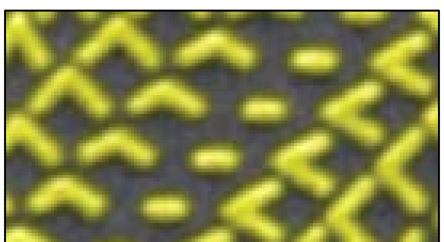


Computational Materials Sciences

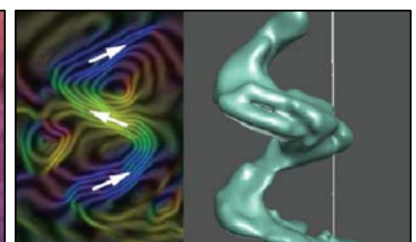
in support of the Materials Genome Initiative

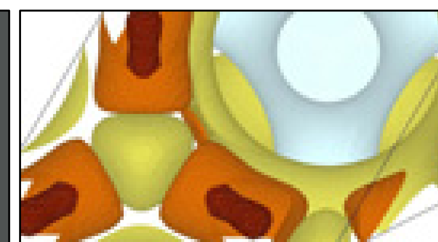
Deliverable: Open-source community codes and software packages that incorporate multiple length and time scales for discovery and prediction of materials functionality

- Deliver research codes and data for design of functional materials to the materials sciences communities in academia, labs, and industry
- Use integrated teams combining expertise in materials theory, modeling, computation, synthesis, characterization, and processing/fabrication
- Use facilities and tools for materials synthesis, characterization, simulation, and computation, relying especially on the SC scientific user facilities
- $8 M in support for multiple teams will begin in FY 2015 for planned 4-years award terms.
- Funding level per Application: $2 M to $4 M per year for 4 years (due date 04/17/2015)


Tailored Surfaces for Advanced Electronics


Novel Thermal Transport


Next Generation Magnets

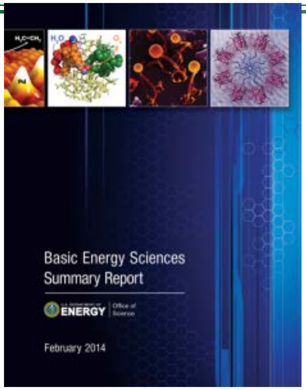

Enhanced Light Absorption

More Information - BES On-line Publications

BES 2014 Summary Report

http://science.energy.gov/bes/research/

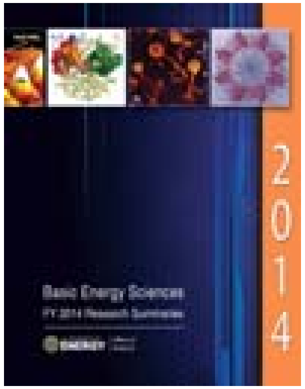
- Overview of BES
- How BES does business
- Descriptions and representative research highlights for 3 BES divisions, EFRCs, and Energy Innovation Hubs



BES FY 2014 Research Summaries

http://science.energy.gov/bes/research/

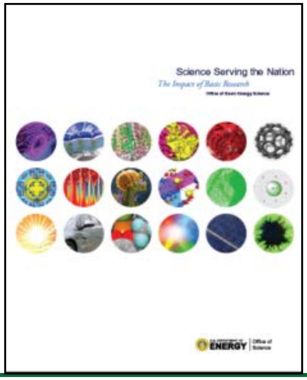
- Summaries of more than 1,200 research projects at some 200 institutions across the U.S.



Science Serving the Nation

http://science.energy.gov/bes/benefits-of-bes/

- Brief vignettes describing the impact of BES funded research on scientific innovation and its impact on end-use technology

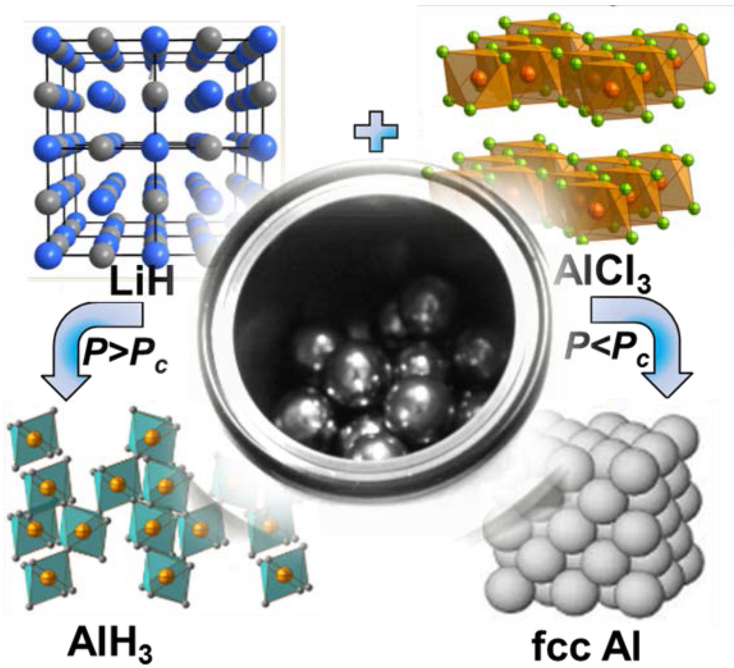


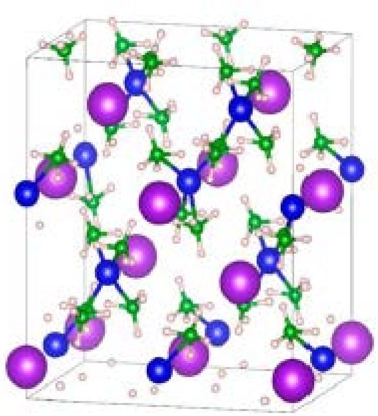
BES PI Participation in 2015 AMR

Hydrogen and Fuel Cells – Hydrogen Storage

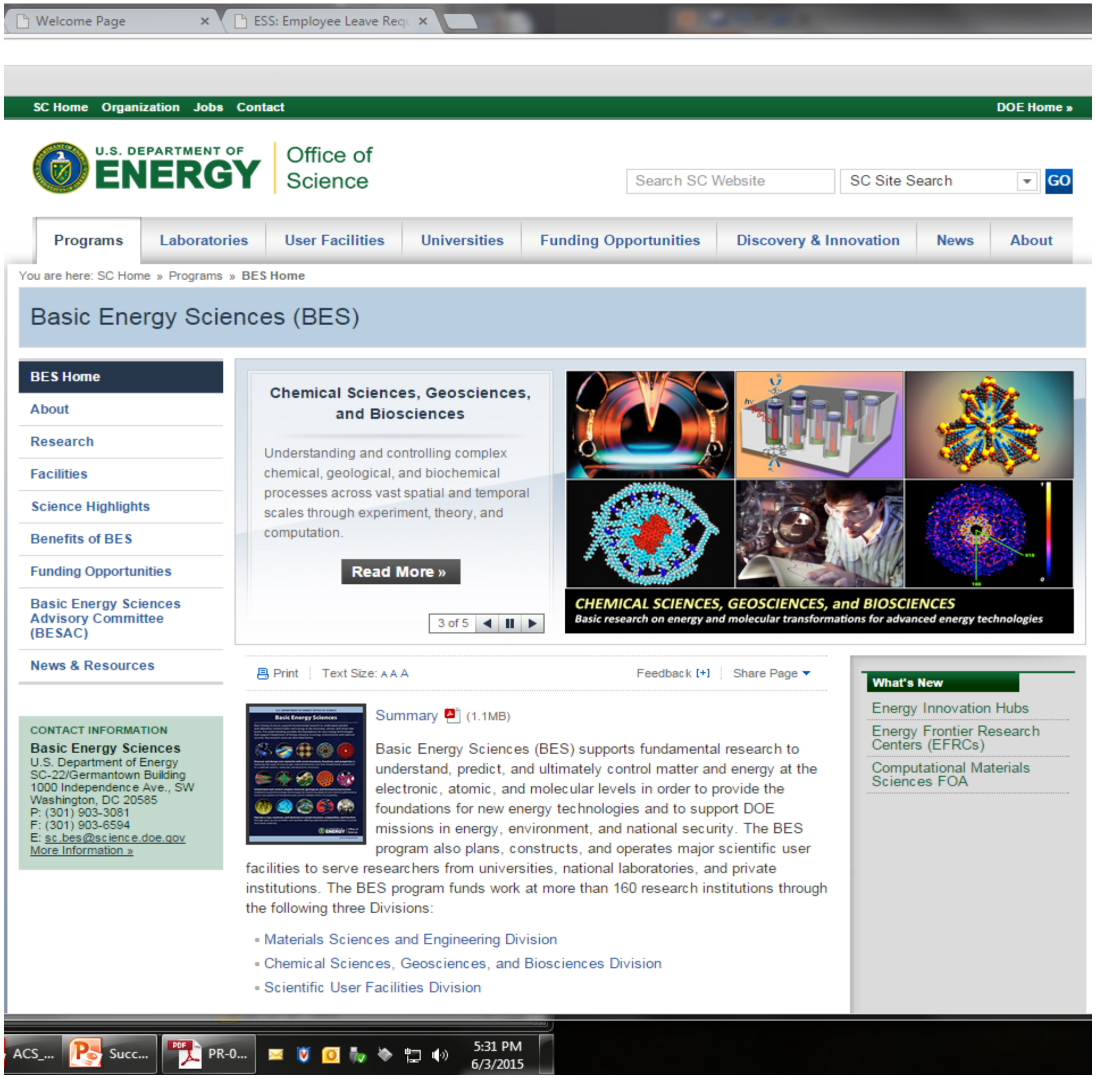
- Presentations: Wed., June 10; 4:15 – 5:45
  Crystal Gateway Salon H

- Posters: Wed., June 10; 6 – 8 pm
  (Grand Ballroom)





Questions? For more information --



http://science.energy.gov/bes/