Basic Energy Sciences Update

Annual Merit Review

Hydrogen & Fuel Cells Program and Vehicle Technologies Program

June 16, 2014

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

DOE Office of Science: 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

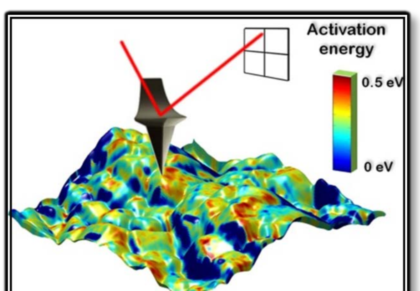
Supporting:

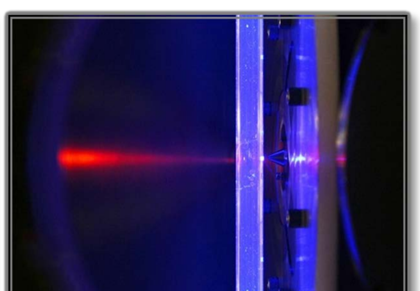
- Energy Frontier Research Centers
- Fuels from Sunlight & Batteries and Energy Storage Hubs
- The largest collection of facilities for electron, x-ray, and neutron scattering in the world

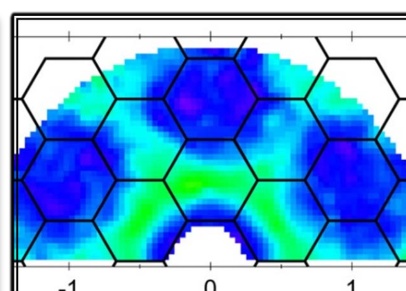
The Scientific Challenges:

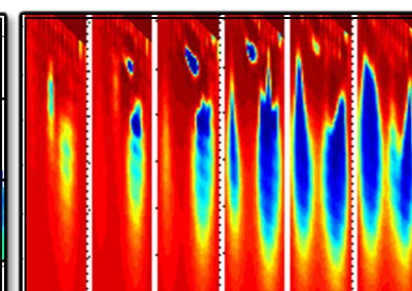
- Synthesize, atom by atom, new forms of matter with tailored properties, including nano-scale objects with capabilities rivaling those of living things
- Direct and control matter and energy flow in materials and chemical assemblies over multiple length and time scales
- Explore materials & chemical 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

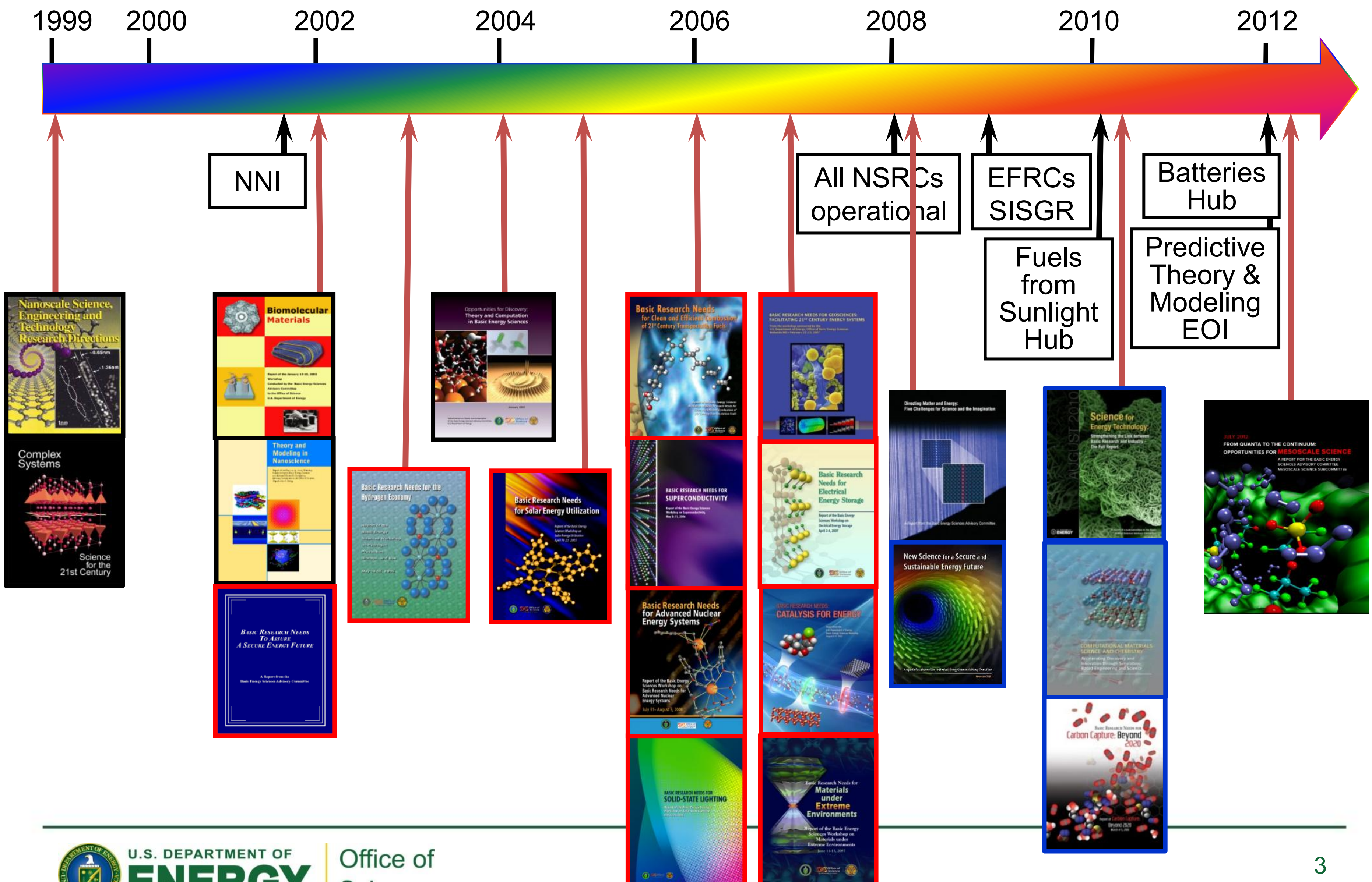






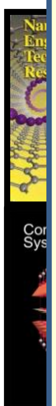


Timeline of BES Strategic Planning and Program Development:

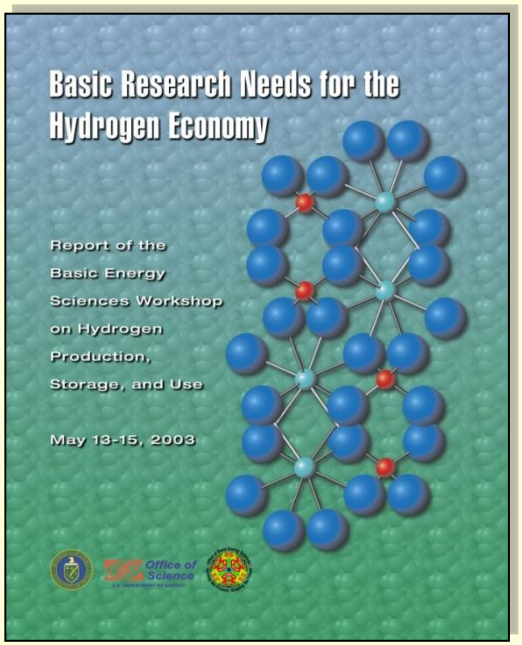


Timeline of BES Strategic Planning and Program Development:

1999 2000 2002 2004 2006 2008 2010 2012

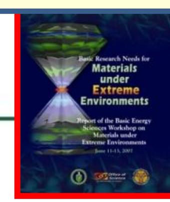


Basic Research R&D Plan: BES Hydrogen Workshop Report



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."



BES Research Activities

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 (46)**
  Research centers, established in 2009 ($2-5 million/year), engage in fundamental research related to topics described in the Basic Research Needs workshop reports.

- **Energy Innovation Hubs (2)**
  Research centers, 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.

Quantum Chemistry and Engine Performance

Scientific Achievement

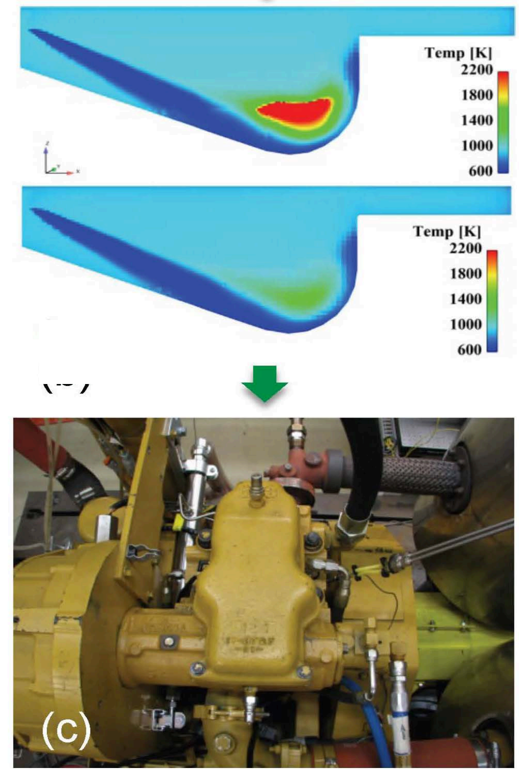
The role of individual molecular reaction rates in combustion engines was assessed via computer simulations of the combustion of a model biodiesel fuel, examining how quantum chemistry affects predictions of high fidelity combustion simulations

Significance and Impact

An understanding of the individual reaction rates and associated quantum chemistry can lead to more accurate and detailed models for engine design and optimization

Research Details

- Combustion simulators have typically not included the underlying chemical detail of combustion processes, potentially missing important molecular-level quantum mechanical effects
- A three-dimensional model was developed that included detailed descriptions of the chemistry of a surrogate for a biodiesel fuel, as well as all the features of the engine
- Key Finding: Quantum tunneling corrections for the rate of the reaction $HO_2 + HO_2 = H_2O_2 + O_2$ were found to have a noticeable impact on performance of a high-fidelity model of a diesel engine



Top: A cut through the cylinder showing the spatial distribution of temperature for different treatments of tunneling; Bottom: Caterpillar single-cylinder test engine

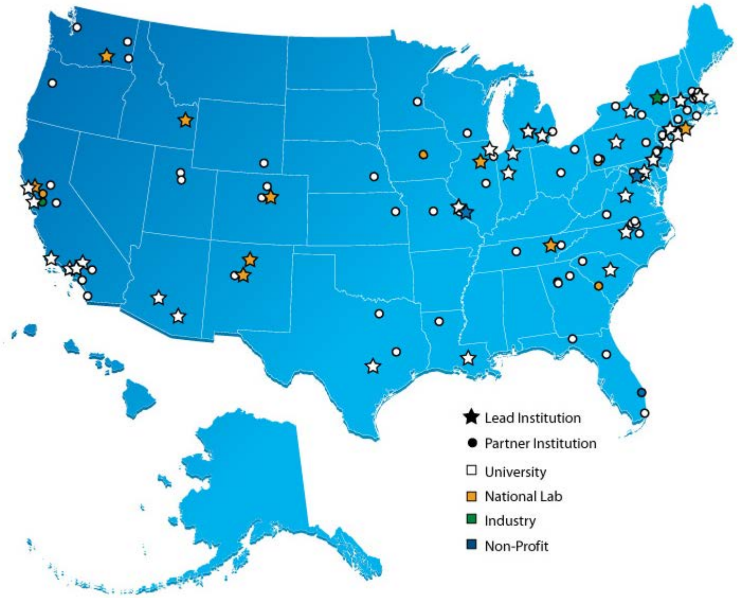
M.Som et al J. Phys. Chem. Lett. **4**, 2021 (2013) [DOI: 10.1021/jz400874s]
J. Zhou et al, J. Phys. Chem. A **116**, 2089 (2012) [DOI: 10.1021/jp209684s].

Energy Frontier Research Centers

46 EFRCs were launched in late FY 2009; $777M for 5 Years

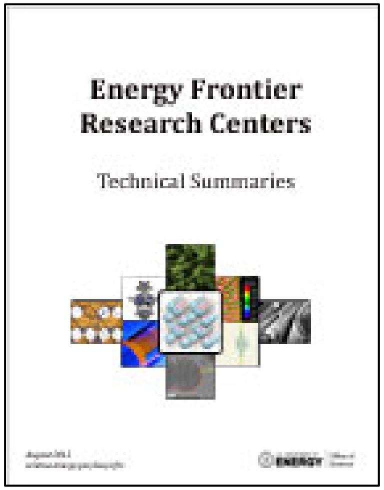
Participants:

- 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 (~4.5 years funding):

- >5,400 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

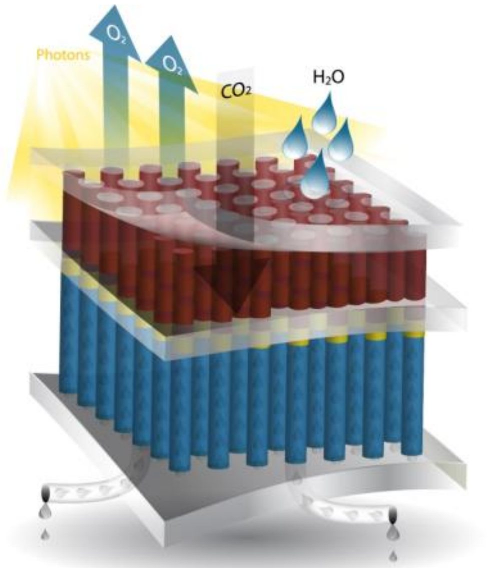


http://science.energy.gov/bes/efrc/

Companies that Benefit from EFRC Research

AltaDevices
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
thermaura
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
Exxon
Mobil
Millifluidica
Pioneer
Dow
Delphi
Spero
NanoFlex Power Corporation
Corning
Ford
Toyota
Gentherm
Micromidas
Semprius
Konica Minolta
Sharp
Invista
NanoIntegris
SiNode Systems
Proton On Site
Polyera
Oorja
LanzaTech
NanoVoltaics
Remylop Structured Materials
QuantumScape
QD Vision
Primet Precision Materials
Orthogonal
nohms Technologies
NEXT

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



Research Accomplishments:
- Accelerated discovery of light absorbers and catalysts via unique high-throughput synthesis and electrochemical screening, rapid materials analysis, and data mining.
- First standardized protocol for catalyst evaluation under conditions relevant for solar water splitting, allowing accurate comparisons of large numbers of materials and devices from different sources
- New coatings that increase stability and protect photocathodes and photoanodes from damage, for more efficient fuel production
- Test bed systems to evaluate water splitting components
- Prototype designs including one that enabled continuous hydrogen production under near-neutral conditions

Mission: Develop a solar-fuels generator, from earth-abundant elements, that is scalable to manufacture and uses only sunlight, water, and carbon dioxide for fuel production 10 times more efficiently than current crops.

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

2014 Major Milestone:
- Design the first prototypic devices for testing components as an integrated system

Details:
- Established on Sept. 30, 2010
- Led by Caltech w/ LBNL, SLAC, Stanford, UC Berkeley, UC San Diego, UC Irvine
- 83 publications (plus 13 submitted)
- 18 patent applications and/or invention disclosures
- 201 presentations
- Decision for continued funding beyond the initial term, ending in September 2015, will be made early in FY 2015

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.

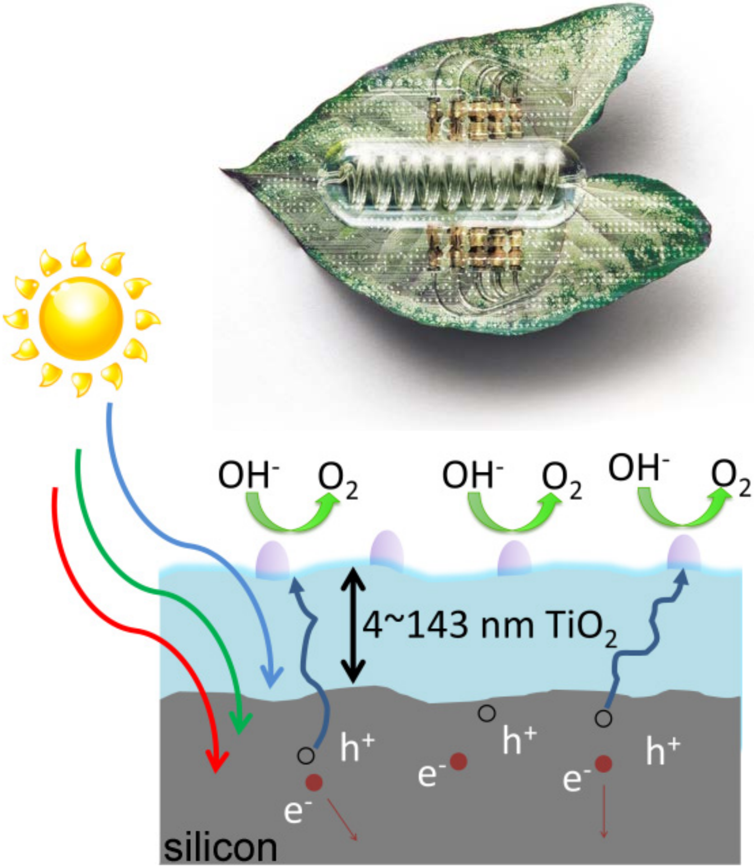
Significance and Impact

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

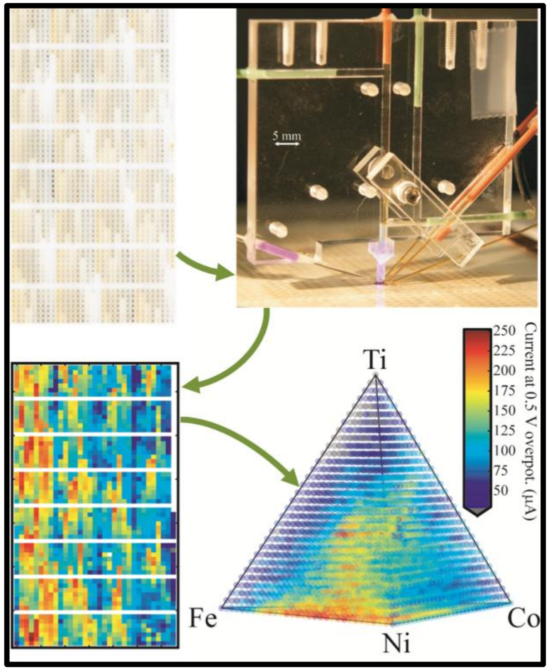
– In conjunction with islands of nickel oxide electrocatalysts, protected silicon can continuously and stably oxidize water for over 100 hours at photocurrents of >30 mA cm^{-2} under 1-sun illumination



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

Cutting-Edge Technology Allows for Rapid Evaluation of Potential Energy-Related Materials



The JCAP-invented high throughput droplet cell scans an array of solutions consisting of multiple variations of a (Fe-Ni-Co-Ti)O_x catalyst. An electrochemical map is produced from the data, which shows the activity of the material as a function of its composition.

Gregoire, J. M. et al. *Rev. Sci. Instrum.* (2013) 84: 024102. DOI: 10.1063/1.4790419

Scientific Achievement

Novel cell design allows high throughput electrochemical and photochemical screening to aid materials discovery, for instance in the discovery of electrocatalysts for hydrogen or oxygen evolution.

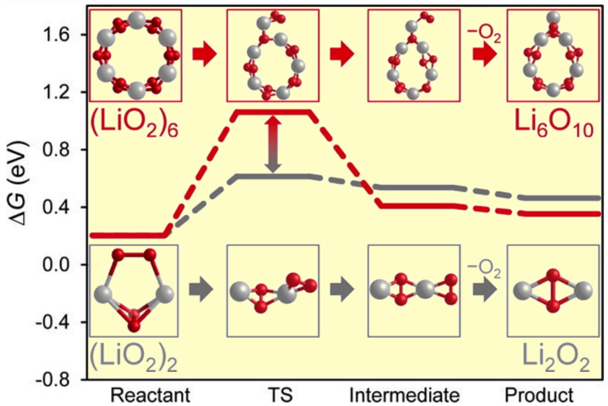
Significance and Impact

High throughput (photo)electrochemical characterization of arrays of candidate materials, a.k.a. material libraries, can be used to identify the most promising materials for solar energy generation.

Research Details

- Rapid scanning techniques are required to develop materials for water splitting.
- A new cell design allows high-throughput scanning of candidate materials and catalysts.
- Materials of various compositions can be arranged into libraries for analysis.
- The newly designed cell technique can rapidly perform many (photo)electrochemical characterizations of materials to determine the most promising ones for solar energy generation.

Joint Center for Energy Storage Research



Reaction pathways for LiO_2 reduction to Li_2O_2 in Li-O_2 batteries, *Das et al, J Phys Chem Lett 5, 813 (2014)*

Research Accomplishments:

- Molecular design and test of high-performance Li_2S cathodes
- Infinite current collector: percolating networks of nanoscale conductors improve charge transfer kinetics in liquid electrodes (patent applied for)
- Techno-economic modeling of alternate designs for lithium-air batteries
- Prediction of chemical pathways for Li-O_2 batteries (left)
- Molecular design and test of new electrolyte for Mg battery
- In-situ observation of dendritic SEI formation from Li electrolytes

Vision: Transform transportation and the electricity grid with high performance, low cost energy storage

Mission: Deliver electrical energy storage with five times the energy density and one-fifth the cost within five years

Legacies

- Library of fundamental knowledge
- Research prototype batteries for grid and transportation
- New paradigm for battery R&D

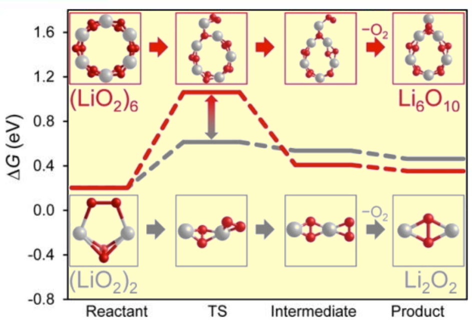
Initial Milestones:

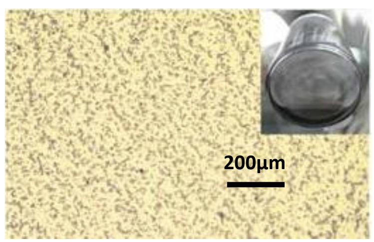
- Electrolyte Genome generates data for >500 organic solvents
- State-of-the-art Electrochemical Discovery Lab designed
- Mg-ion and flow battery research prototypes launched

Background:

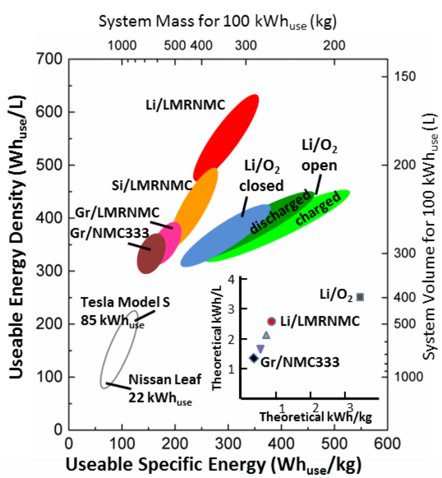
- New paradigm: incorporate Discovery Science, Battery Design, Research Prototypes and Manufacturing Collaboration in one highly interactive organization
- Launched December 2012
- Led by George Crabtree (ANL) with national laboratory, university and industrial partners: LBNL, SNL, SLAC, PNNL,UIUC, NWU, UChicago, UIC, UMich, Dow, AMAT, JCI, CET
- State of Illinois provided $5M (of $35M commitment) for a new JCESR building with state-of-the-art laboratory and meeting space (site selected and design underway).

JCESR – First Year Scientific Highlights





Fine-grained structure of improved cathodes



- **Predicting Chemical Pathways for Li-O_2 Batteries**

  Predictions for the structure and molecular conversion pathways in the discharge reaction $LiO_2 \rightarrow Li_2O_2$ were made using high level quantum chemical theory; these discoveries are being used to guide strategies to optimize the energy density, reversibility, and efficiency for Li-O_2 batteries

- **Molecular Design Leads to Record Performance for Li_2S Cathodes**

  Record performance for Li_2S cathodes was demonstrated for cathodes with an innovative molecular design based on density functional theory - Tests showed a 40% increase in capacity over 500 cycles and only half the polysulfide loss after 20 cycles compared to conventional binders

- **Techno-economic Modeling of Li-Air Batteries**

  Techno-economic modeling (“building battery systems on the computer”) of alternate designs for lithium-air batteries (with General Motors) compares their performance and cost to other possible next-generation batteries concluding that lithium-air batteries are unlikely to meet stringent volume requirements of electric vehicle applications. The material-to-system analysis informs strategic directions for JCESR’s discovery science, battery design and research prototyping

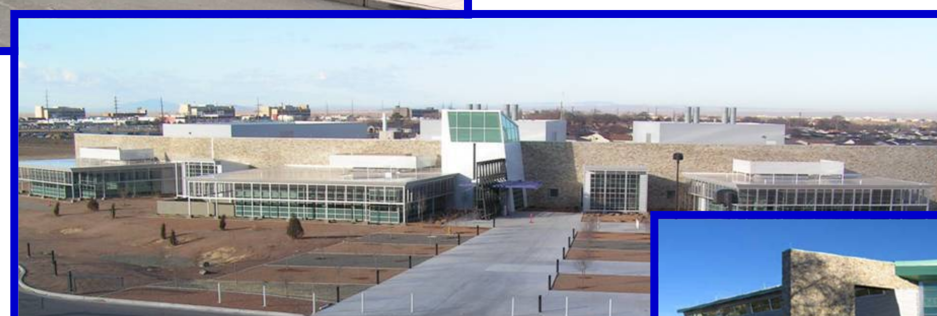
BES Nanoscale Science Research Centers—
Completed in 2006 – 2008, Serving >2000 users/Yr

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)

Capabilities at the Nanoscale Science User Facilities

- Advanced synthesis of nanoscale materials
  - Clean room fabrication including lithography
  - Atomically controlled synthesis
- Wide range of characterization techniques
  - Microscopy, NMR, spectroscopy, etc.
- Specialized analytical tools
  - Discovery platforms (SNL CINT)
- Theory, Modeling and Simulation
- Coupled to x-ray and neutron scattering facilities
- Specialized capabilities for biological systems
  - Deuteration for neutron scattering (ORNL CNMS)
  - Biological imaging

Visualizing and Understanding Reaction Paths in Lithium-ion Batteries

Scientific Achievement

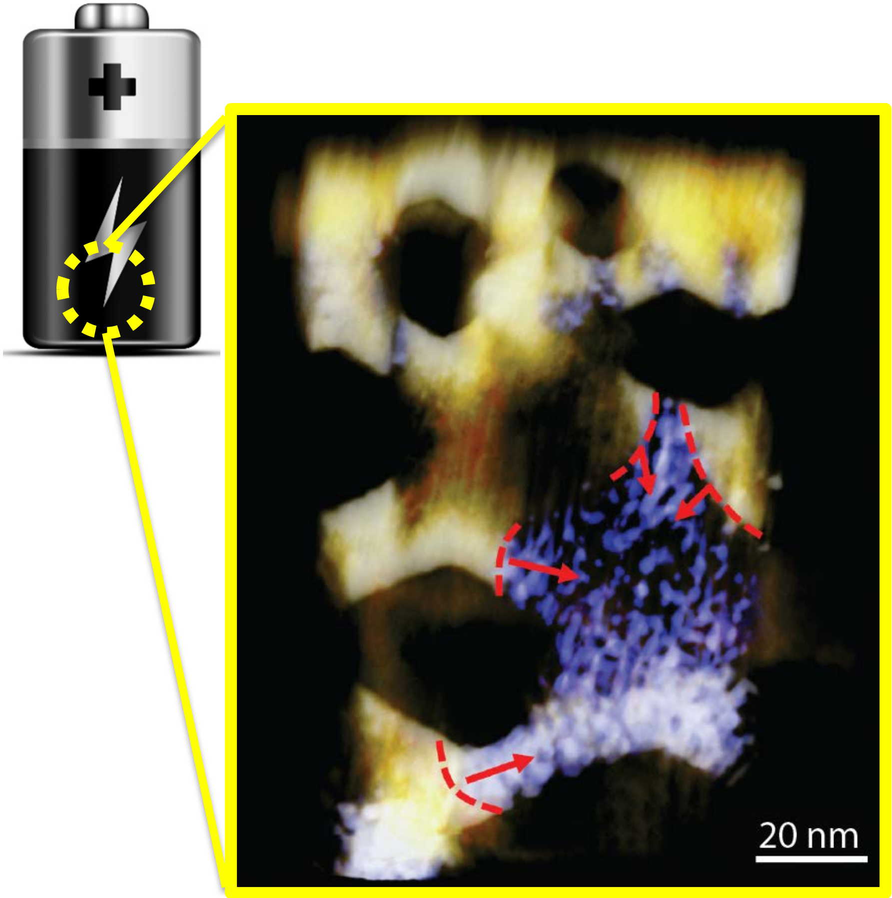
Scientists are exploring new electrode materials to satisfy the ever increasing demand for batteries with larger energy storage capacity. To evaluate and improve these materials, they must be "seen" in action, while the battery is charging or discharging. This CFN-led collaboration developed a novel method that uses x-rays and electron microscopy to visualize the changes that occur during the charging of an electrode. The images reveal how a nickel oxide anode in a Li-ion battery is chemically transformed into metallic nickel during the charging process.

Significance

1. This novel experimental approach facilitates the probing of the properties of electrodes in real batteries.
2. The results shed light onto the origin of the inhomogeneous charge distribution in battery electrodes and will stimulate ways of improving battery performance.
3. The visualization method can be used to understand and assess many other electrode materials.

CFN Capability

The Electron Microscopy Facility at CFN provided high resolution transmission electron microscopy.



Heterogeneous phase conversion is dominant during the charging and discharging of nickel oxide (NiO) nanosheets within a lithium ion system. The contours and arrows in the image highlight the edges of the regions where the phase converted and the direction of the phase conversion that simultaneously propagated in a single NiO nanosheet..

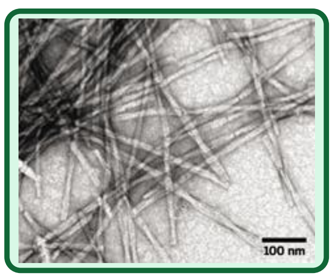
F Lin, D. Nordlund, TC Weng, Y. Zhu, C. Ban, RM. Richards, HL Xin, *Nature Communications* **5**, 3358, 2014.

Examples of Industry Use of NSRCs

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.

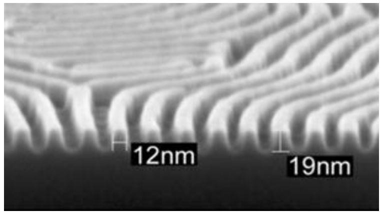


TMF

HGST a Western Digital company

Ultradense Memories

Expertise in polymer nanostructure self-assembly and electron microscopy can be applied to Terabit/cm2 scale magnetic memories for computing and imaging

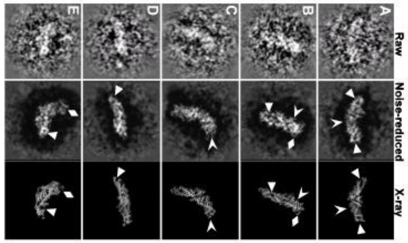


CFN

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



TMF

3M

High Performance Fuel Cells

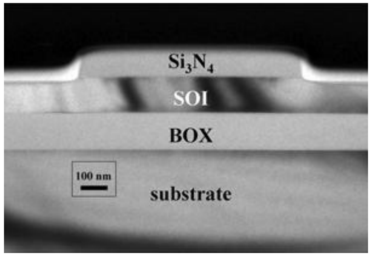
Understanding limitations to new Nanostructured Thin Film (NSTF) catalyst activity to improve Performance and durability of fuel cells

CNMS/ShaRE

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.



CNM

FY 2015 BES Budget Request

Research programs

- Energy Innovation Hubs & Energy Frontier Research Centers are funded at FY 2014 levels
- Core Research approximately flat with FY 2014
- Computational Materials Sciences ($24.2M)

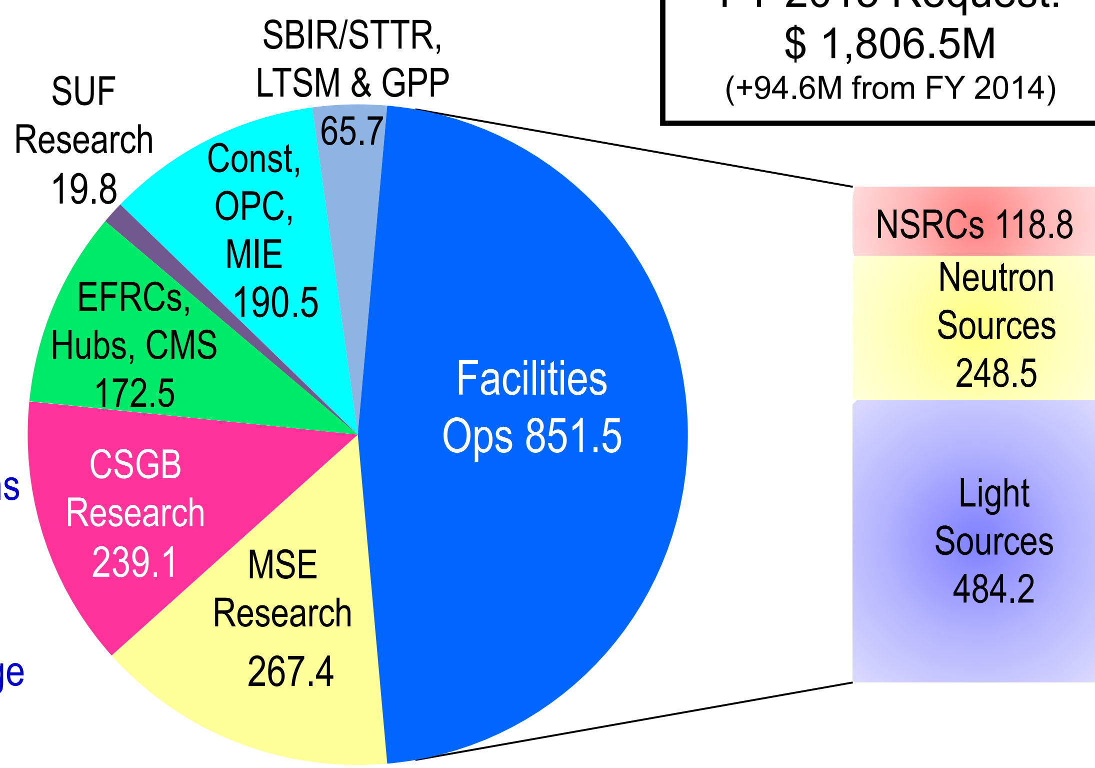
Scientific user facilities

- All full operating facilities at optimal operations
- NSLS-II transition to full operations ($115M)
- NSLS & Lujan cease operations; funding requested to transition facilities to safe storage

Construction and instrumentation

- NSLS-II instrumentation (NEXT) ($22.5M)
- Advanced Photon Source upgrade ($20M)
- Linac Coherent Light Source-II ($138.7M + $9.3M OPC)

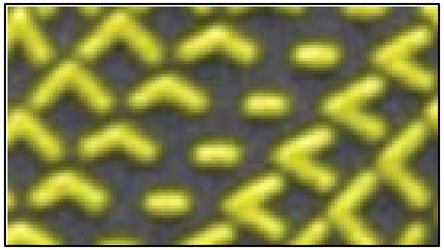
FY 2015 Request:
$ 1,806.5M
(+94.6M from FY 2014)



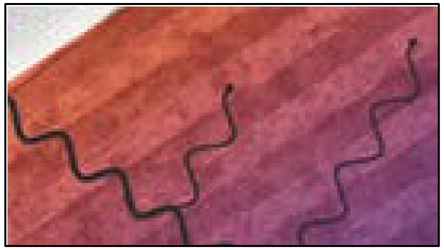
Computational Materials Sciences
Accelerating Materials Discovery and Development

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

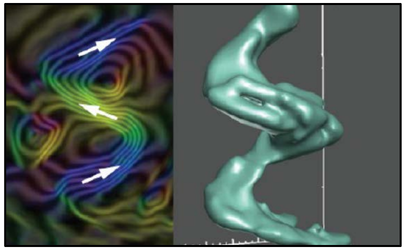
- Deliver research codes and data for design of functional materials to the materials sciences communities in academia, labs, and industry
- Use integrated teams combining expertise in materials theory, modeling, computation, synthesis, characterization, and processing/fabrication
- Use facilities and tools for materials synthesis, characterization, simulation, and computation, relying especially on the SC scientific user facilities
- Support will begin in FY 2015 for up to 4 teams for multi-year awards



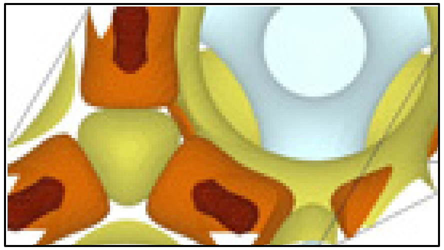
Tailored Surfaces for Advanced Electronics



Novel Thermal Transport

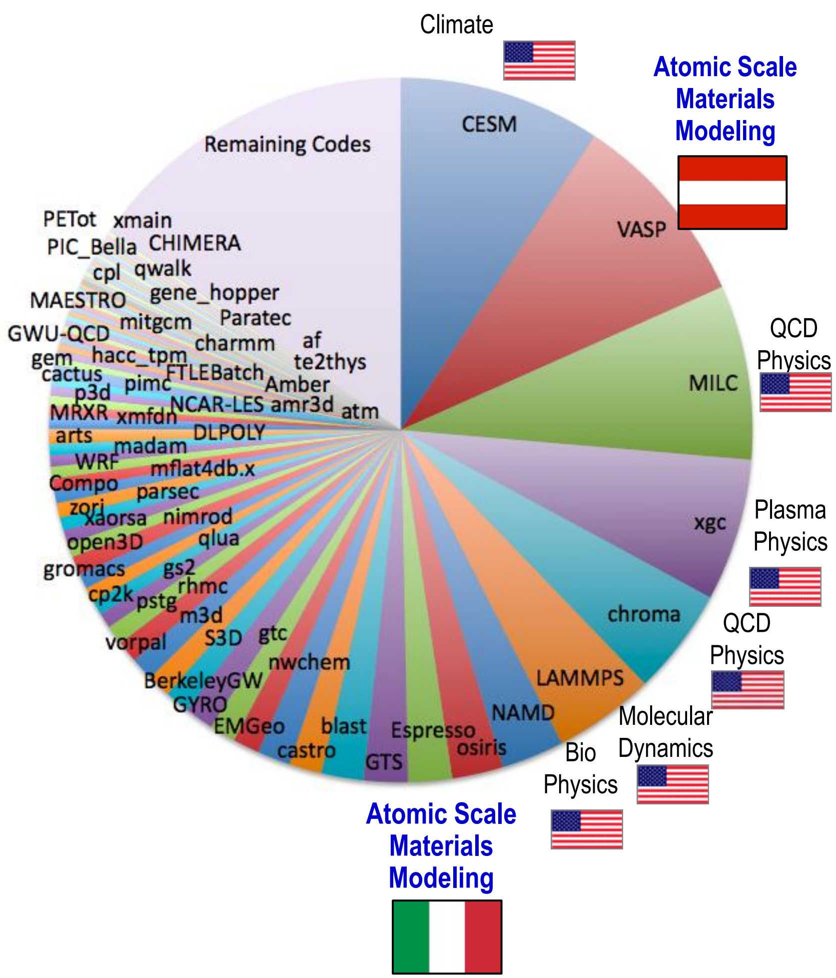


Next Generation Magnets



Enhanced Light Absorption

Software is Key to US Leadership in Materials Sciences



2012 Top Application Codes at NERSC

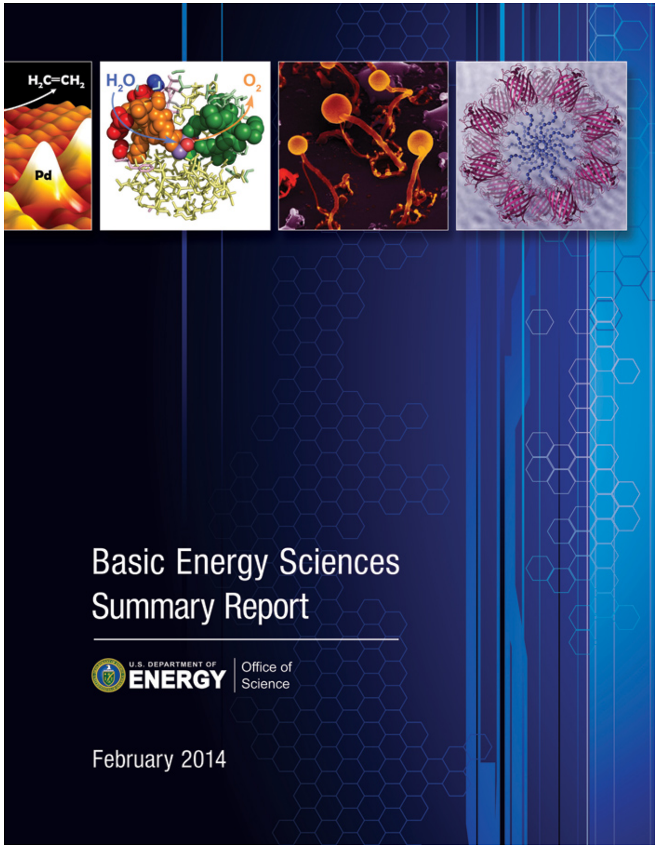
Today – US trails Europe in computational codes for materials discovery and engineering

- For materials users at NERSC, the most used code is VASP
  - Atomic scale materials modeling
  - Commercial code (users have to have their own purchased license) from Austria
- 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.
- Another materials software package in wide use in over 70 countries to calculate thermodynamic data, largely in metals, is Thermo-Calc
  - From Sweden, commercially available for 25 years

Future – US-developed materials sciences software can inform future development of high performance computing, including the path to exascale

BES Program Summary

- **BES 2014 Summary Report**
  - Update to the 2011 Summary Report
  - Overview of BES
  - How BES does business
  - Descriptions of all three BES divisions, EFRCs, and Hubs
  - Representative research highlights from the BES divisions, EFRCs, and Hubs



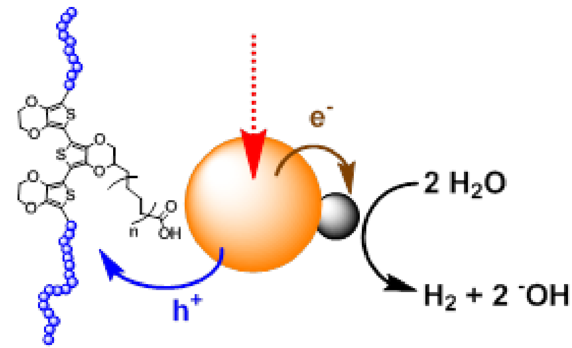
- **BES Core Research Activities (CRAs)**
  - Updated to reflect current portfolio descriptions, accomplishments, and challenges

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

BES PI Participation in 2014 AMR

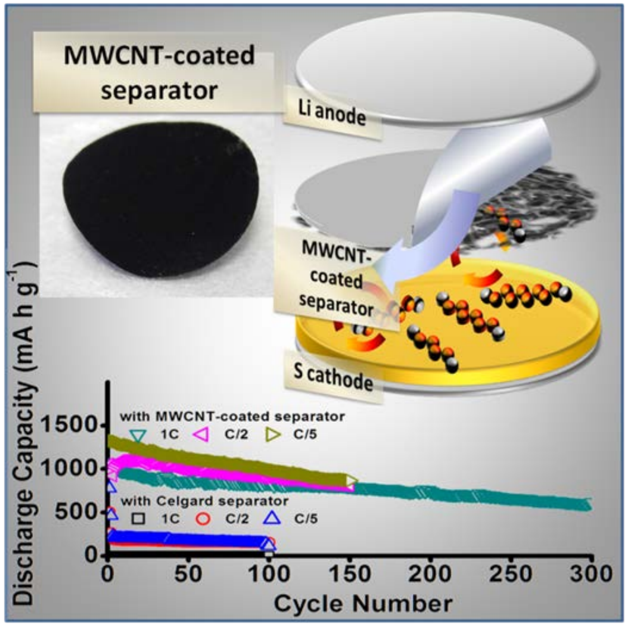
Hydrogen and Fuel Cells – Hydrogen Production

- Presentations: Wed., June 18; 2:15 – 6:15
  Thurs., June 19; 1:45 – 4:45
  (Roosevelt 1)
- Posters: Thurs., June 19; 6 – 8 pm
  (Exhibit Hall B)



Energy Storage for Vehicles

- Posters: Mon., June 16; 6 – 8 pm
  (Exhibit Hall A)



Questions? For more information --