U.S. DEPARTMENT OF ENERGY | Office of Science

Basic Energy Sciences Overview

Annual Merit Review

Fuel Cell Technologies Program and Vehicle Technologies Program

May 14, 2012

Dr. Linda Horton

Director, Materials Sciences and Engineering Division

Office of Basic Energy Sciences

Secretary
Steven Chu

Deputy Secretary
Daniel B. Poneman

Advanced Research Projects Agency – Energy
Arun Majumdar

Under Secretary for Nuclear Security/Administrator for National Nuclear Security Administration
Thomas P. D'Agostino

- Defense Nuclear Nonproliferation
- Defense Programs
- Naval Reactors
- Counter-terrorism
- Defense Nuclear Security
- Emergency Operations

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Patricia Dehmer

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- **High Energy Physics** — James Siegrist
- **Advanced Scientific Computing Research** — Dan Hitchcock
- **Nuclear Physics** — Tim Hallman
- **Biological & Environmental Research** — Sharlene Weatherwax
- **Fusion Energy Sciences** — Ed Synakowski
- **SBIR/STTR** — Manny Oliver
- **Workforce Develop. for Teachers & Scientists** — Pat Dehmer (A)

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- Energy Efficiency & Renewable Energy — David Danielson
- Fossil Energy — Charles McConnell
- Nuclear Energy — Pete Lyons
- Electricity Delivery & Energy Reliability — Pat Hoffman

Basic Energy Sciences

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

The Program:

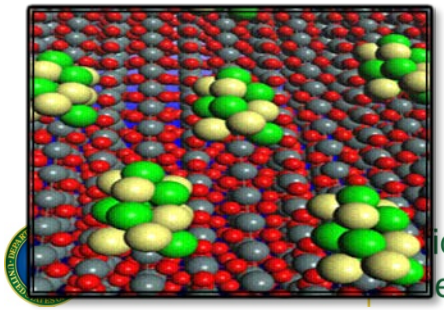
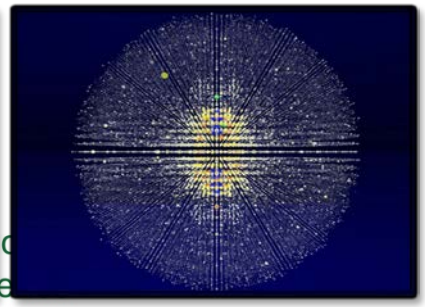
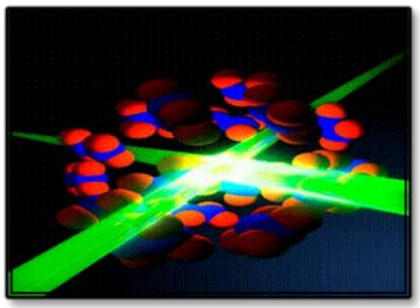
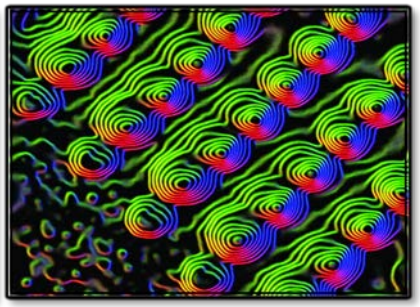
Materials sciences & engineering—exploring macroscopic and microscopic material behaviors and their connections to various energy technologies

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

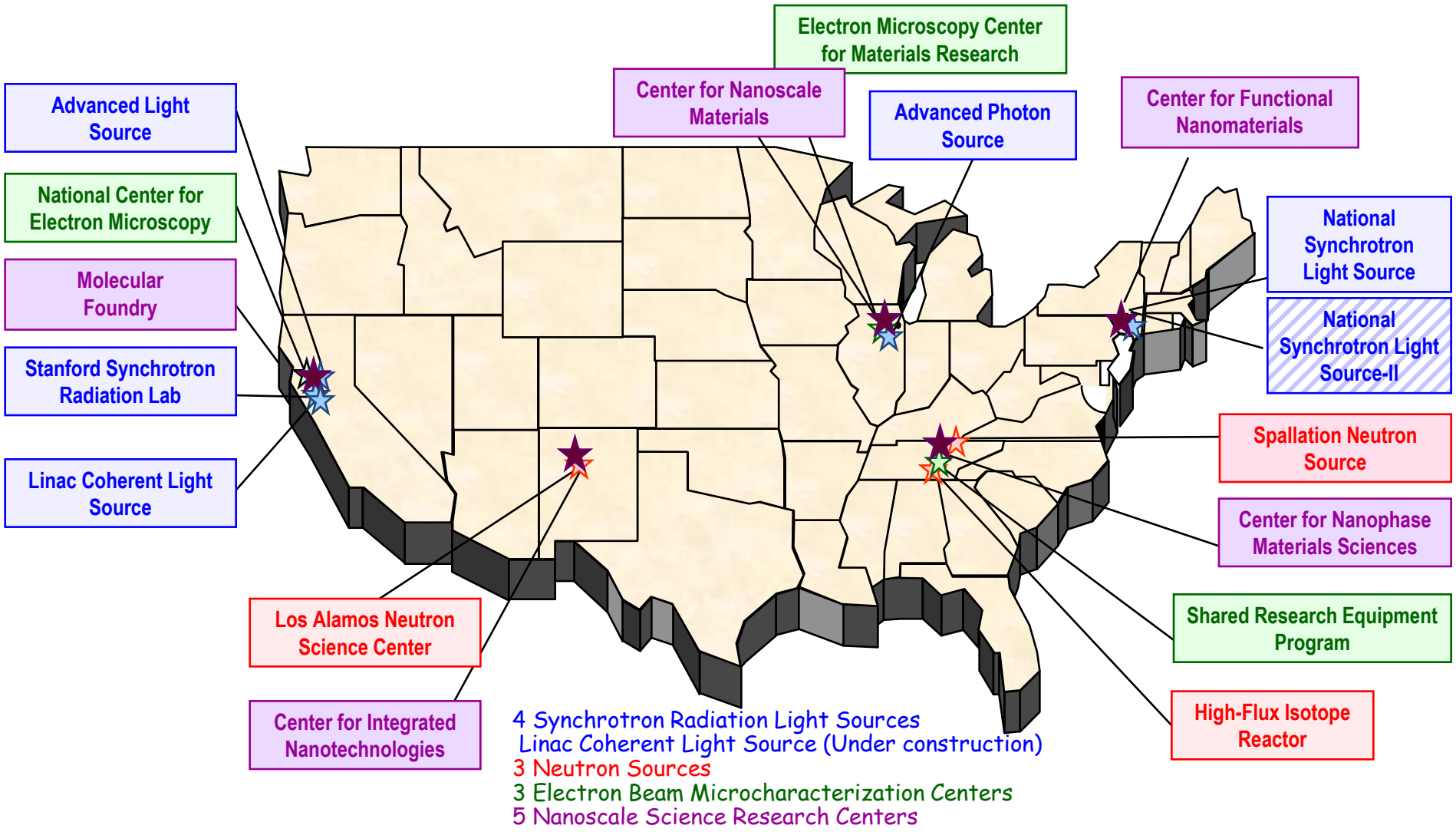
Supporting:
- 46 Energy Frontier Research Centers
- Solar Fuels Hub
- The largest collection of facilities for electron, x-ray, and neutron scattering in the world

The Scientific Challenges:

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

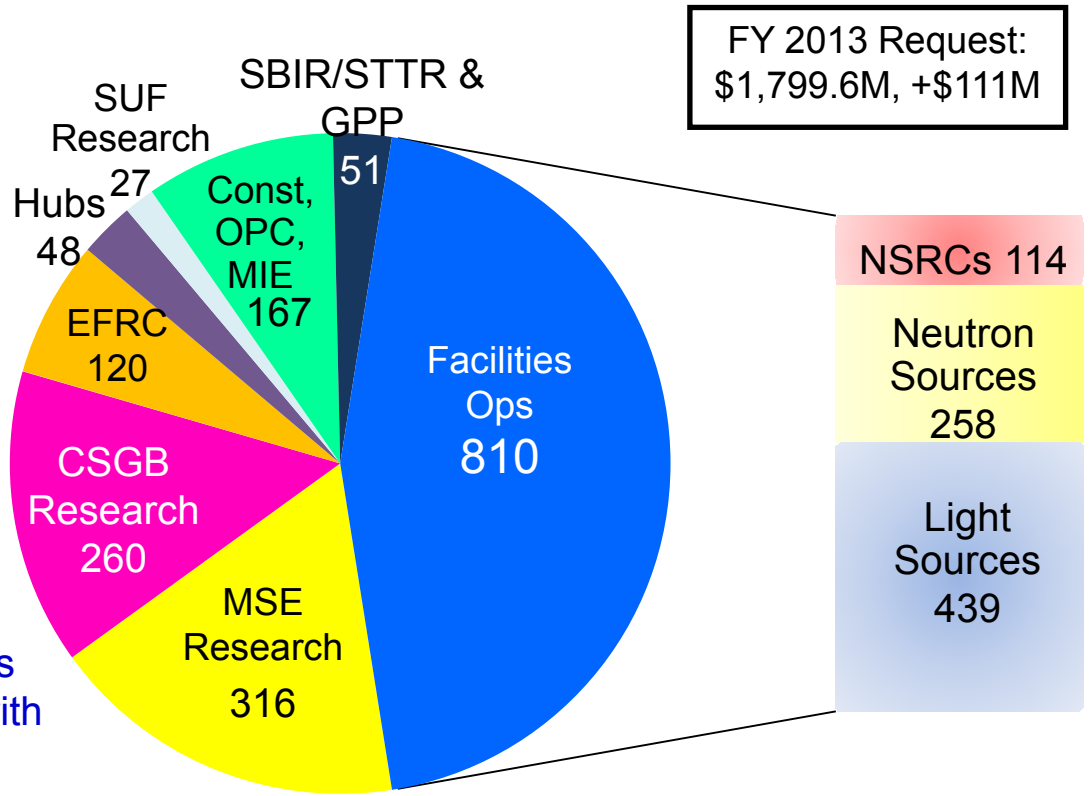





BES Scientific User Facilities
Transforming the Discovery Process



FY 2013 BES Budget Request

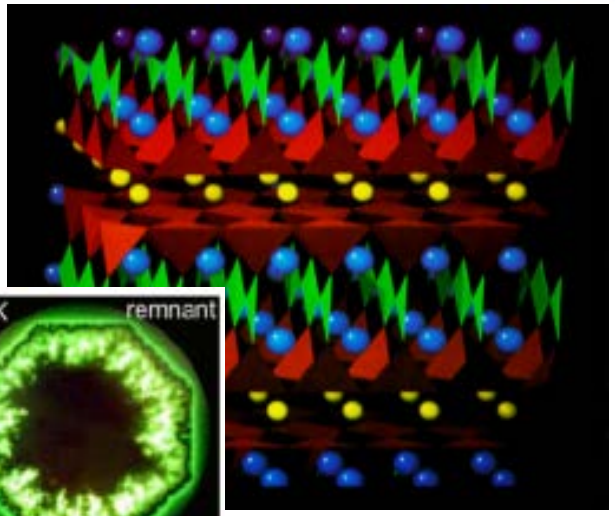
- Research programs
  - Energy Innovation Hubs (+$5M)
  - Energy Frontier Research Centers
    - Joint EERE R&D (+$20M)
  - Core Research
    - Materials and Chemistry by Design (+$20M)
    - Science for Clean Energy (+$42M)
- Scientific user facilities operations
  - Near optimum operations of all facilities (+$42M)
    - Synchrotron light sources
    - Neutron scattering facilities
    - Nanoscale Science Research Centers
  - Instrumentation for clean energy, joint with EERE (+$15M)
  - NSLS-II Early Operations (+$22M)



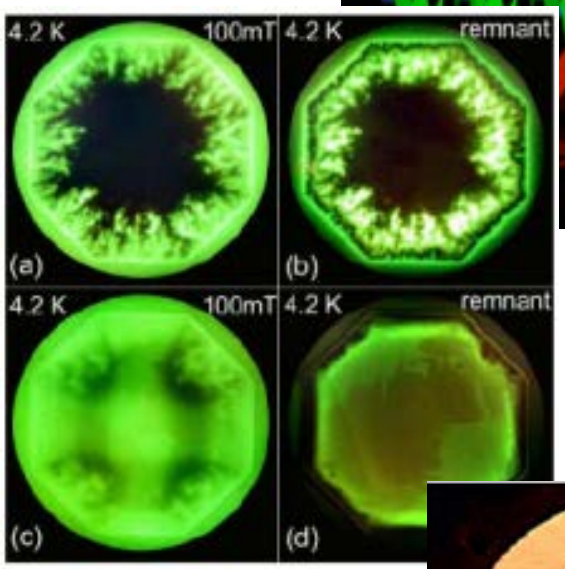
- Construction and instrumentation
  - National Synchrotron Light Source-II
  - NSLS-II instrumentation (NEXT) ($12M)
  - Advanced Photon Source upgrade ($20M)
  - Linac Coherent Light Source-II ($64M)

Science for Clean Energy: Nanoscale to Mesoscale Sciences

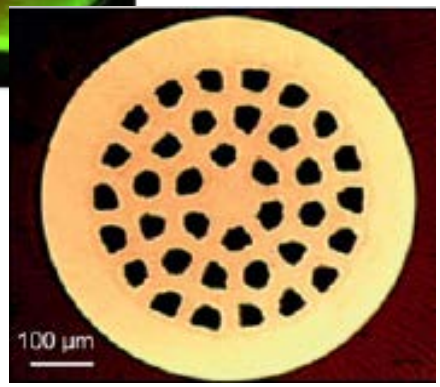
- Developing the next generation of materials, chemicals, and game-changing processes—understanding structure, properties, and function from atoms and molecules, through the nanoscale, and to the mesoscale (+$42M).
- Research will enable science-based chemical and materials design and manufacturing in, for example:
  - direct conversion of solar energy to fuels
  - generation of electricity from clean energy sources
  - storage and transmission of electrical energy
  - carbon capture, utilization, and sequestration
  - the efficient use of energy
- Collaboration with the Office of Energy Efficiency and Renewable Energy will accelerate the transition of scientific discoveries into prototype clean energy technologies (+$20M).



First determination of the structure of the high Tc super-conductor $YBa_2Cu_3O_{7-x}$ determined using neutron scattering.



Magneto-optical images of superconducting films

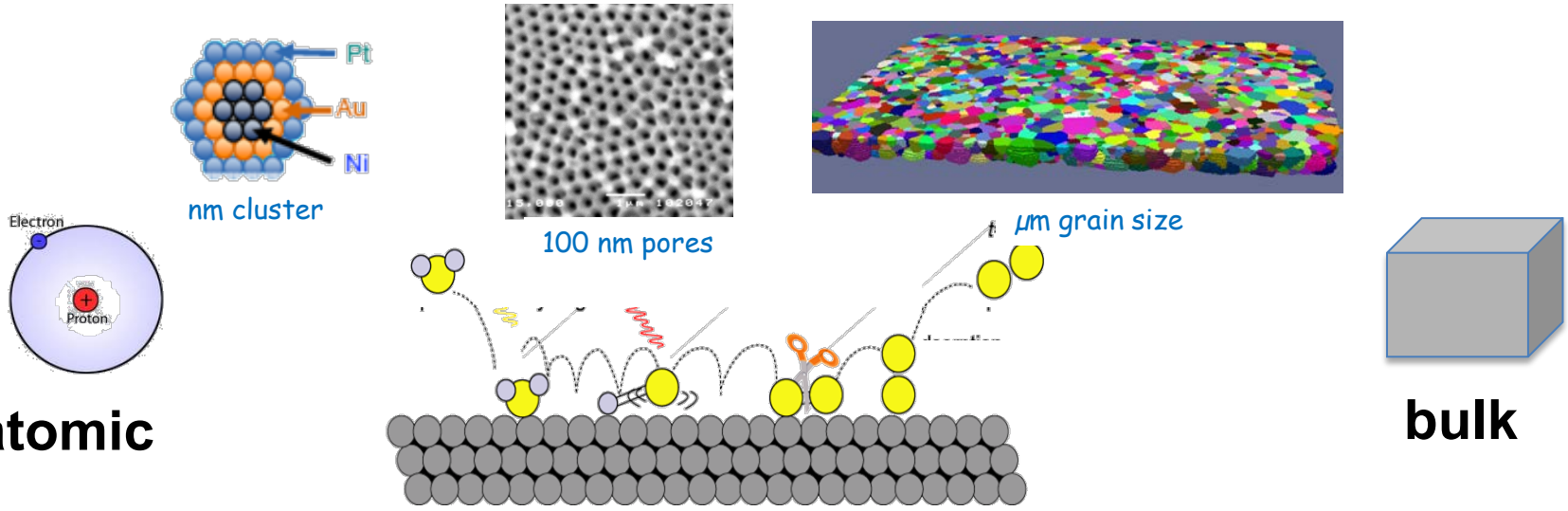


Fabricated industrial wires of MgB_2 superconductors used in MRIs and commercial magnets.

Nanoscale and Mesoscale Sciences

A path to enabling manufacturing innovations

Structure, Dynamics, Function



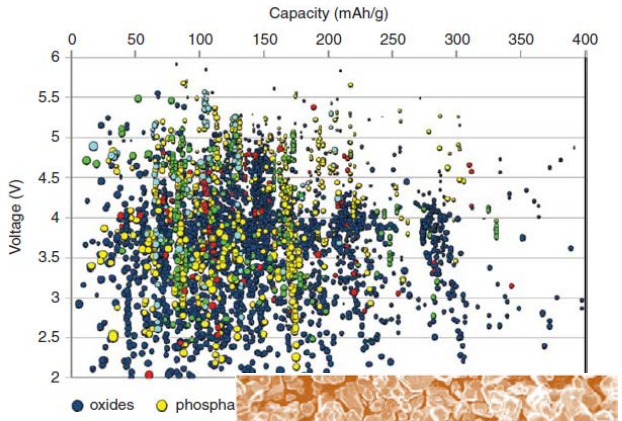
Visionary Outcomes:

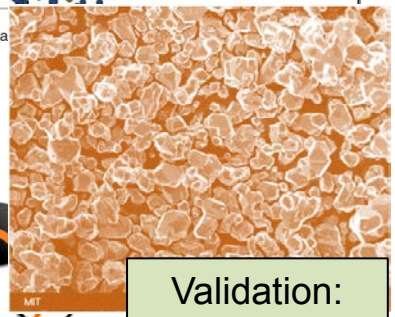
- Complexity and functionality of biology with inorganic earth abundant materials
- Systems with many degrees of freedom; new organization principles
- Paradigm shift from top down design with classical building blocks to bottom up design with atomic, molecular and nano components

Materials and Chemistry by Design
Accelerating Discovery for Global Competitiveness

- Research to establish design rules to launch an era of predictive modeling, changing the paradigm of materials discovery to rational design (+$20M).
  - New software tools and data standards to catalyze a fully integrated approach from material discovery to applications
- Discovery of new materials has been the engine driving science frontiers and fueling technology innovations. Research would utilize the powerful suite of tools for materials synthesis, characterization, and simulation at DOE's world-leading user facilities
- Integrated teams to focus on key scientific knowledge gaps to develop new theoretical models
  - Long-term: realization in reusable and broadly-disseminated software
  - Collection of validated experimental and modeling data for broader community use

Prediction: New battery materials starting from first principles theory





Validation: Materials fabrication

MATERIALS PROJECT

http://materialsproject.org/

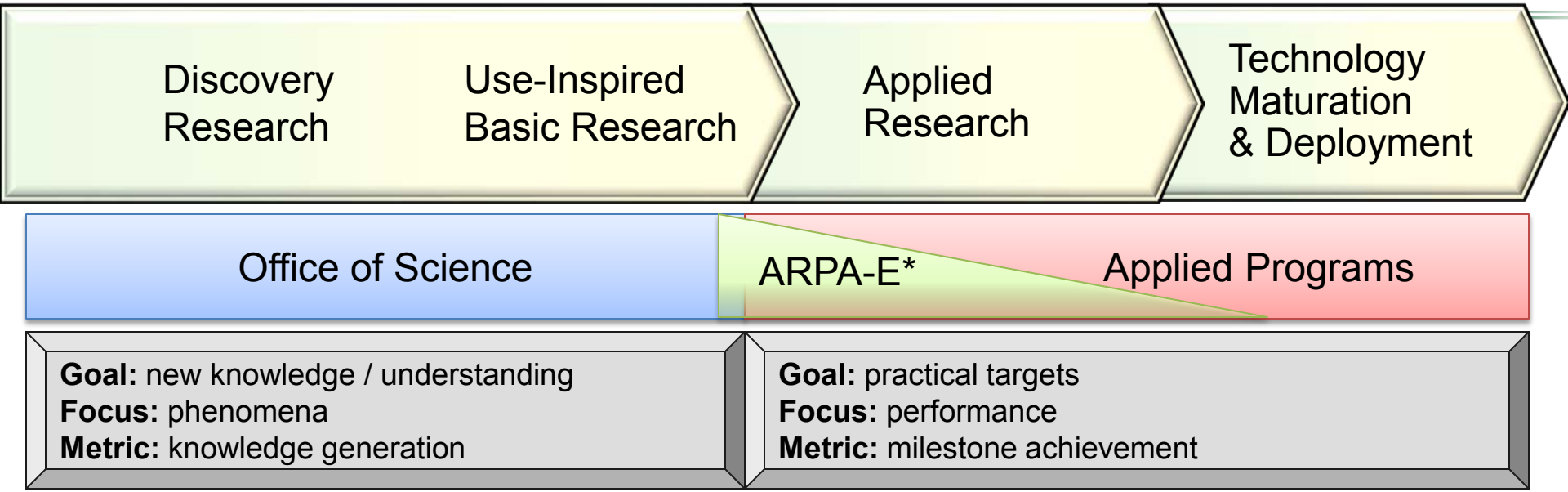
End Use: Software on-line for general community use

BES Research — Science for Discovery & National Needs

Increasing progression of scientific scope and level of effort

- **Core Research (many)**
  Support single investigator and small group projects to pursue their specific research interests
- **Energy Frontier Research Centers (46)**
  $2-5 million-per-year research centers, established in 2009, focus on fundamental research related to energy
- **Energy Innovation Hubs (Across DOE, 2 managed by BES)**
  $20 million+ -per-year research centers focus on integrating basic & applied research with technology development to enable transformational energy applications

Continuum of Research, Development, and Deployment

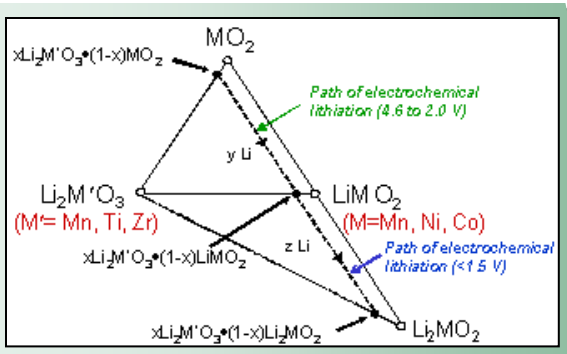


- Basic research to address fundamental limitations of current theories and descriptions of matter in the energy range important to everyday life – typically energies up to those required to break chemical bonds.
- Basic research for fundamental new understanding on materials or systems that may revolutionize 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

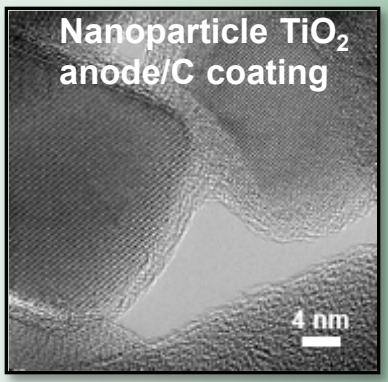
* ARPA-E: targets technology gaps, high-risk concepts, aggressive delivery times

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

Basic Science



Discovered new composite structures for stable, high-capacity cathodes

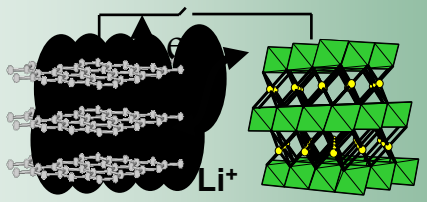


EFRC research

Tailored electrode-electrolyte interface using nanotechnology

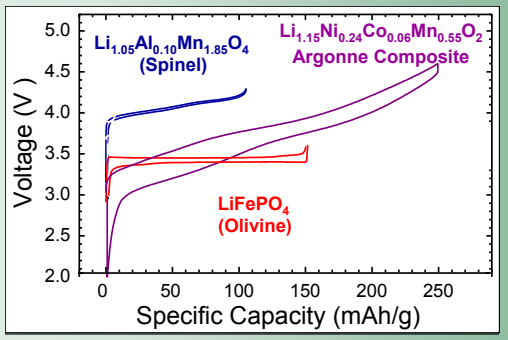
Applied R&D

Li_xC_6 (Anode) **$xLi_2MnO_3•(1-x)LiMO_2$ (Cathode)**



Created high energy Li-ion cells…

…with double cathode capacity, enhanced stability



Manufacturing/ Commercialization

ENVIA SYSTEMS

BASF The Chemical Company

TODA KOGYO CORP.

LG Chem

GM VOLT

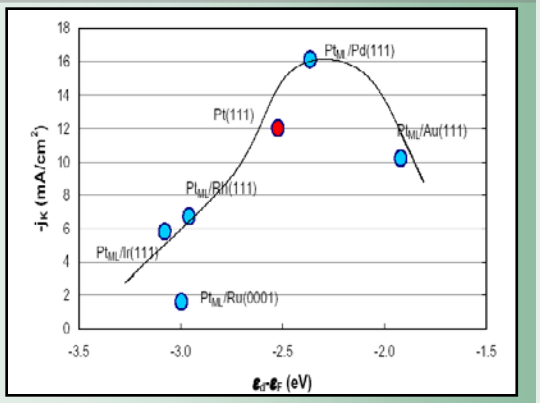
Licenses to materials and cell manufacturers and automobile companies

Platinum Monolayer Electro-Catalysts:
Stationary and Automotive Fuel Cells

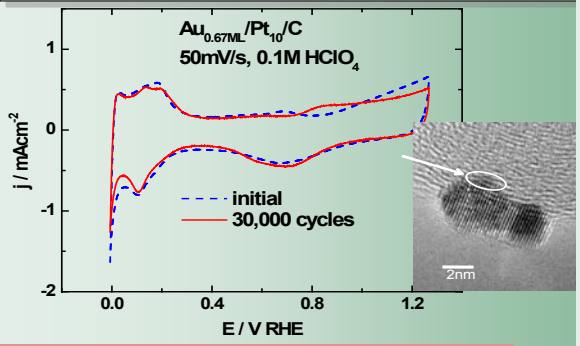
Basic Science | Applied R&D | Manufacturing/ Commercialization

BES
Two research advances

Pt core-shell nano-catalysts: high activity with ultralow Pt mass



Pt stabilized against corrosion in voltage cycling by Au clusters

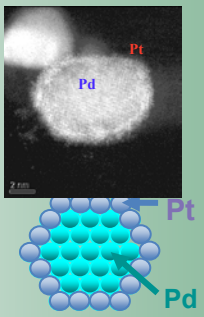


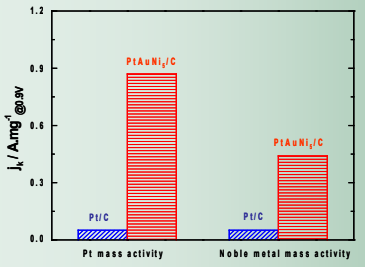
Science **315**, 220 (2007)

BES → EERE
Core-Shell Nanocatalysts

Active Pt ML shell – Metal/alloy core
Core tunes activity & durability of shell

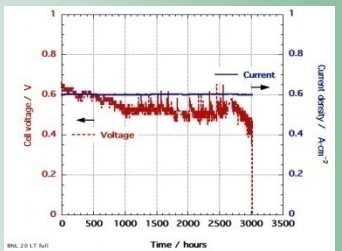
Model and actual image of a Pt Monolayer on Pd nanoparticle





Pt-mass weighted activity enhanced 20x

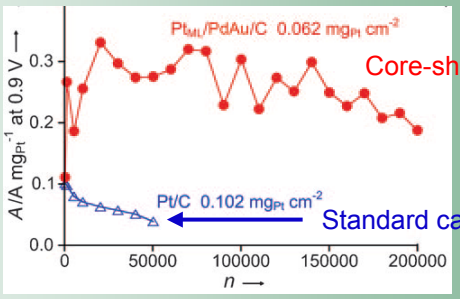
3000 hr Fuel Cell Durability Performance



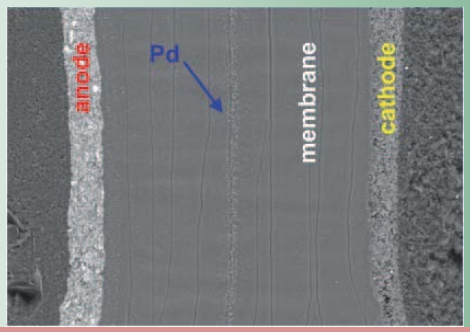
CRADA with Industry

Scale-up synthesis: **Pt-ML/Pd_9Au_1/C**

Excellent fuel Cell durability 200,000 cycles



Membrane Electrode Assembly >200K cycles
Very small Pt diffusion & small Pd diffusion



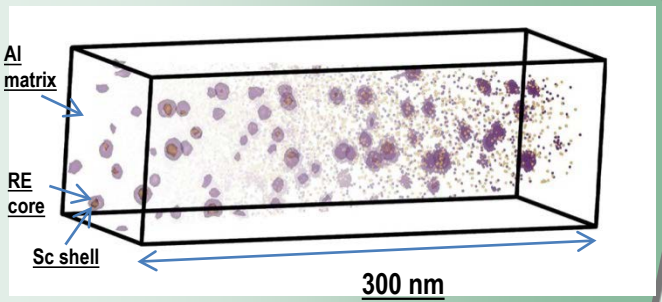
Angewandte Chemie ***49***, *8602 (2010)*

Fuel Cell Catalyst readied for automotive application

New Aluminum Alloys for Energy-Efficient Transportation: from Fundamental Research to Cars and Planes

Basic Science

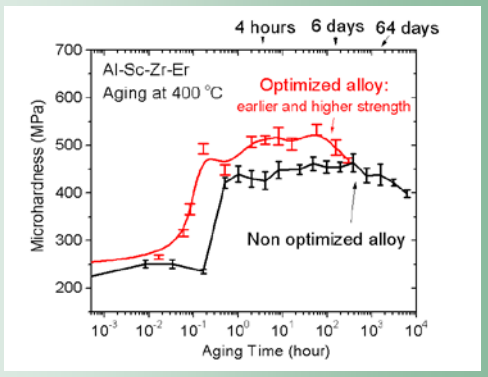
Northwestern University (NU) developed nano-scale precipitates in aluminum, using trace amounts of highly potent, exotic alloying elements: scandium, zirconium, lithium and rare earths (RE).



Information from atomic tomography allows tailoring of precipitate size, spacing, composition and structure, optimizing their strengthening effect and aging resistance.

Applied R&D

Ford and Boeing jointly sponsored applied research at NU to optimize the alloys for energy-efficient airplanes and cars, building on DOE-BES funding.



Optimized properties include strength and resistance to aging at high temperature, manufacturability, and cost. The new alloys can operate at twice the temperature of commercial alloys.

Manufacturing/ Commercialization

New aluminum alloy will be cast into brake rotors and replace much heavier cast-iron rotors, helping Ford improve mileage of its cars.

New aluminum alloy may be used to replace titanium in elevated temperature applications, such as heat shields.

New Catalyst Speeds Conversion of Electricity to Hydrogen Fuel

Scientific Achievement

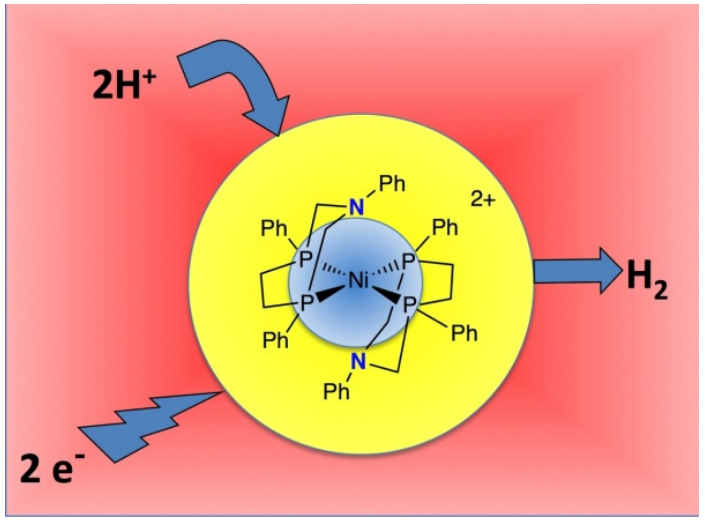
A newly synthesized Nickel complex speeds the production of hydrogen ten times faster than a natural hydrogenase enzyme at room temperature.

Significance and Impact

Opens a new research path to develop long-lived catalysts using inexpensive, earth-abundant metals to convert electrical energy to chemical energy.

Research Details

- In this process, water molecules are split to produce hydrogen and oxygen. Hydrogen can be used as a fuel.
- Using the natural hydrogenase enzyme as a model, a synthetic catalyst using Nickel was developed. The metal atom gets its reactive properties from the groups of atoms containing phosphorous and nitrogen that surround it.
- By splitting water, hydrogen gas is formed by combining the H^+ on the nitrogen with the H^- on the nickel center.
- Adding an acid or water increased the rate of hydrogen produced from the newly-designed synthetic catalyst.



$2\ e^- + 2\ H^+ \rightarrow H_2$

Schematic showing catalyst operation

ML Helm, MP Stewart, RM Bullock, MR DuBois, DL DuBois Science **12 August 2011**: 863. Work was supported by the Center for Molecular Electrocatalysis, an EFRC led by Pacific Northwest National Laboratory.

Proposed Batteries and Energy Storage Hub
Transform the Grid and Electrify Transportation

- The Hub will develop electrochemical energy storage systems that safely approach theoretical energy and power densities with very high cycle life – and have the potential for fundamentally new and economic manufacturing
- These are systemic challenges requiring new materials, systems, innovative engineering, and enhanced scientific knowledge
- The Hub will address key fundamental questions in energy storage including:
  - Can we approach theoretical energy density?
  - Can we safely increase the rate of energy utilization?
  - Can we create a reversible system with minimal energy loss?
  - Can we limit the use of materials that are not earth-abundant?
  - Can we develop totally new battery architectures?
  - Can we enable truly innovative approaches to manufacturing and packaging?
- The Hub will link fundamental science, technology, and end-users, and it will collaborate with relevant BES, Energy Frontier Research Centers, ARPA-E EERE, and OE activities
- Funding Opportunity Announcement Released 2/1/2012; Letters of Intent (required) were due 3/1/2012 and proposals due 5/31/2012

BES Publications for Improved Communication

BES 2011 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 2011 Research Summaries

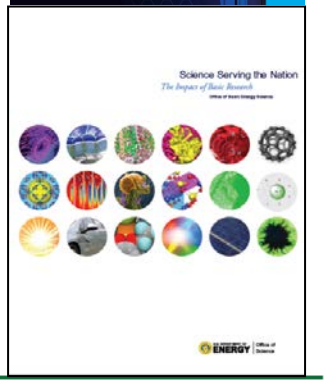
http://science.energy.gov/bes/research/

- Summaries of more than 1300 research projects across 3 BES divisions, including senior investigators, postdocs, graduate and undergraduate students, and a brief project description

Science Serving the Nation

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

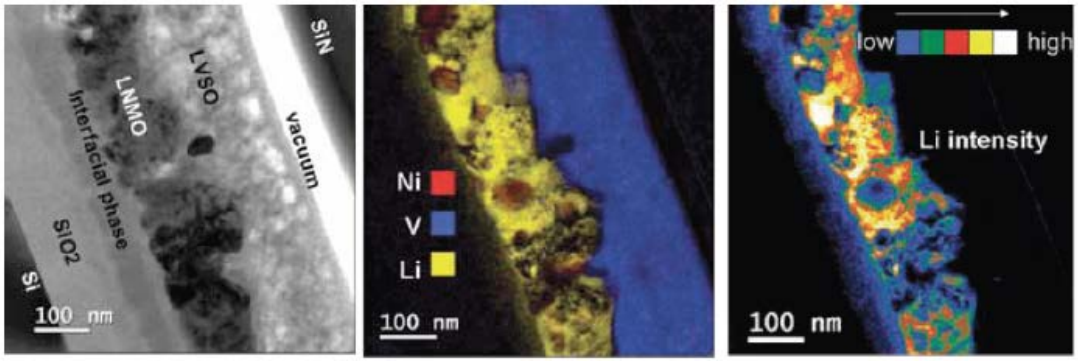
- Brief vignettes describing the impact of BES funded research on scientific innovation and its impact on end-use technology



BES PI Participation in 2012 AMR Meeting

Electrical Energy Storage

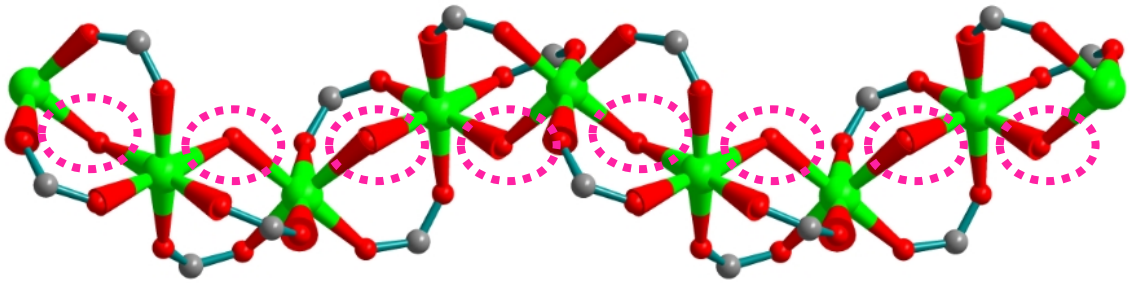
- 23 Poster Presentations (Monday and Tuesday Evening in Crystal Gateway – Grand Ballroom)



TEM micrograph | Ni, V, Li EELS map | Li intensity EELS map

Hydrogen Storage

- 7 Oral Presentations (Wed. 2:15-6:15 pm Crystal Gateway – Salon V)
- 12 Poster Presentations (Wed. Evening in Crystal Gateway – Grand Ballroom)



Questions? – For more information --