U.S. DEPARTMENT OF ENERGY | Office of Science

Fundamental Electrochemical Energy Storage Research

Batteries and Energy Storage Information Meeting

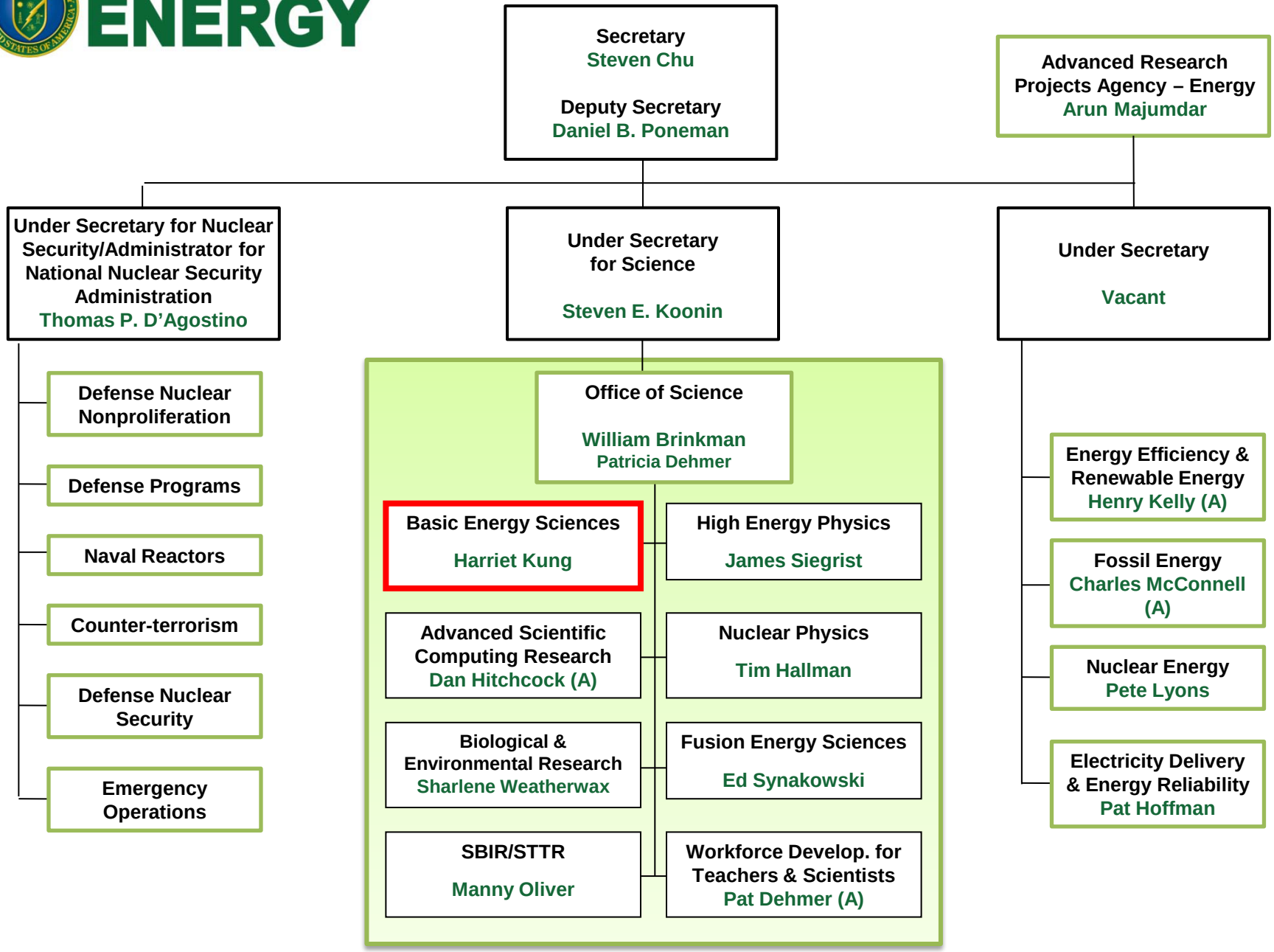
October 21, 2011

John Vetrano

Program Manager and Technical Coordination

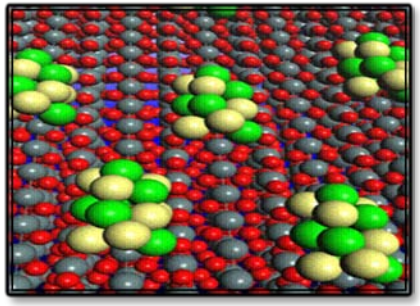
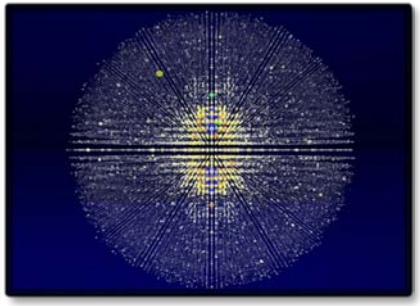
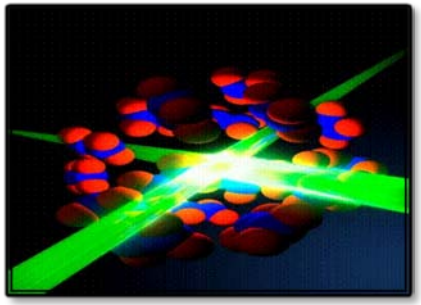
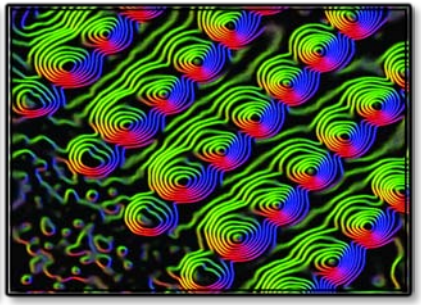
Office of Basic Energy Sciences

U.S. DEPARTMENT OF ENERGY

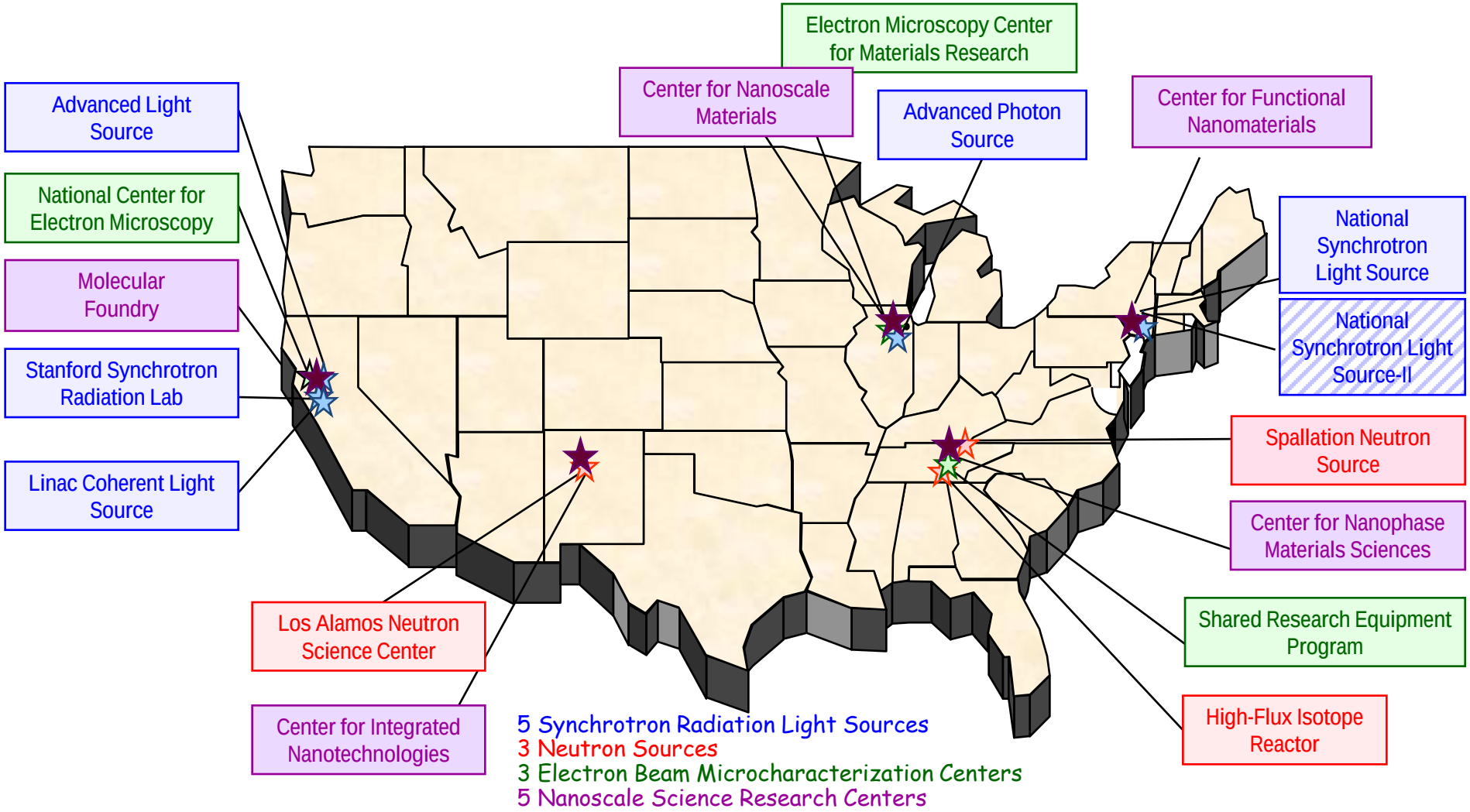


Basic Energy Sciences Mission

- Fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels
- Provide the foundations for new energy technologies to support DOE's missions in energy, environment, and national security
- Plan, construct, and operate world-leading scientific user facilities for the Nation

BES Scientific User Facilities: Resources for Research



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

BES Research — Science for Discovery & National Needs

Three Major Types of Research Thrusts

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)**

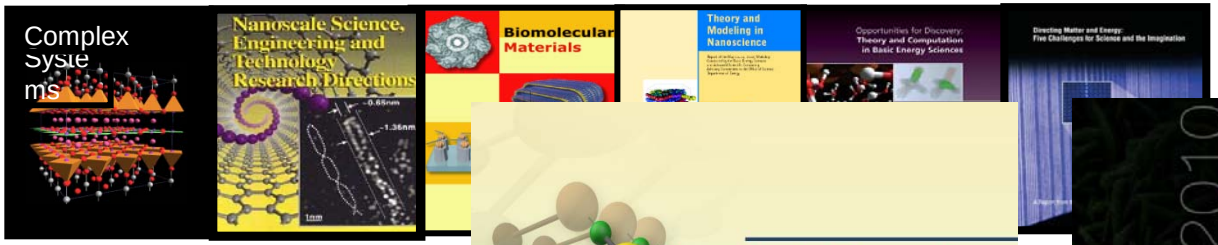
  $2-5 million-per-year research centers, established in 2009, focus on fundamental research related to energy

- **Energy Innovation Hubs (Three Across DOE; Three proposed for FY 2012)**

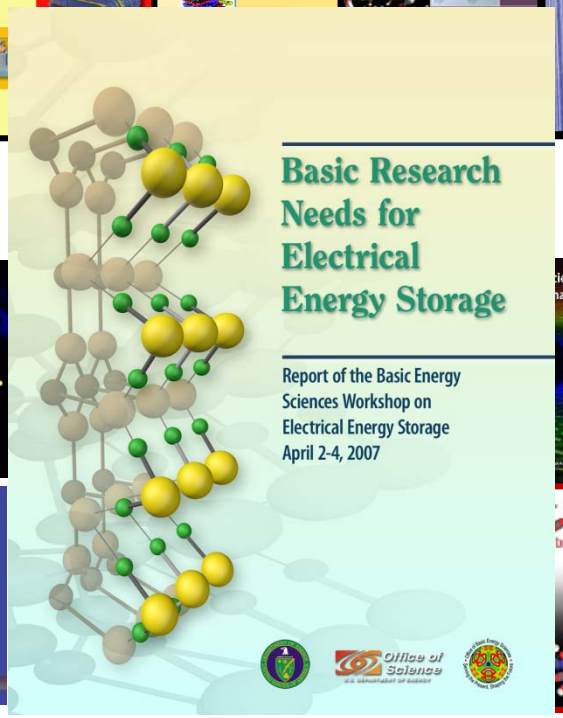
  $20 million+ -per-year research centers focus on integrating basic & applied research with technology development to enable transformational energy applications

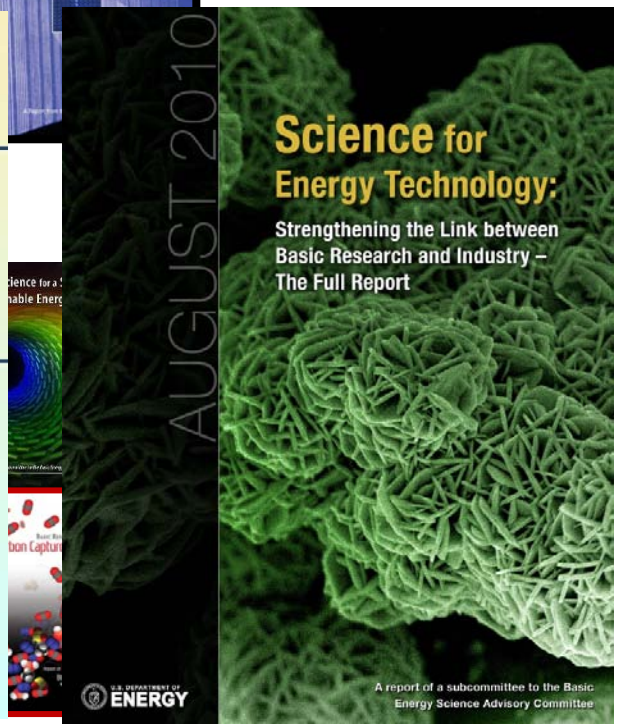
BES Strategic Planning Activities

- *Science for Discovery*

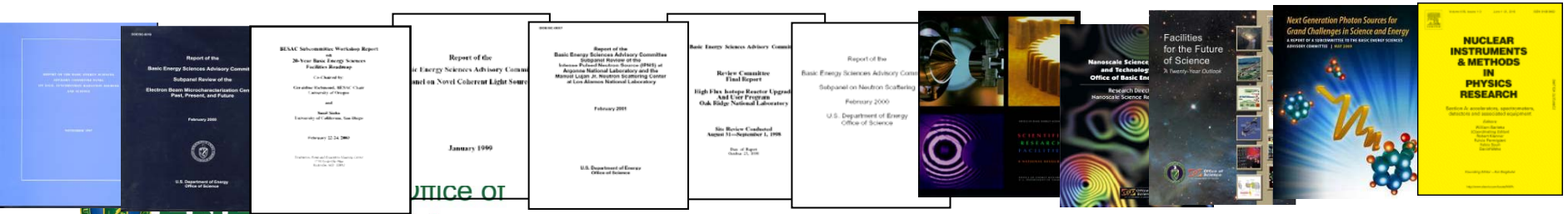


- *Science for National*





- *National Scientific User Facilities, the 21st century Tools of Science & Technology*



Basic Research Needs for Electrical Energy Storage
April 2-4, 2007

Chair: John Goodenough (UT-Austin)
Co- Chairs: Héctor Abruña (Cornell)
Michelle Buchanan (ORNL)

Breakout Session Panel and Leaders:

Chemical Storage Science
- Stan Whittingham, SUNY-Binghamton
- Steven Visco, LBNL

Capacitive Storage Science
- Bruce Dunn, UCLA
- Yury Gogotsi, Drexel

Cross-Cutting
- Daniel Nocera, MIT
- Andy Gewirth, U Illinois

Plenary Session Speakers:

Tien Duong (DOE-EERE) – Transportation Needs
Imre Gyuk (DOE-OE) – Utility Needs
Jean-Marie Tarascon (Univ. de Picardie Julies Verne) – Li-ion Technology, Present and Future
John R. Miller (JME) – Electrochemical Capacitors
Katsuhiko Naoi (Tokyo University of Ag &Tech)) – Advances in Capacitors & Hybrid Devices in Japan

CHARGE: To identify basic research needs and opportunities underlying batteries, capacitors and related technologies, with a focus on new or emerging science challenges with potential for significant long-term impact on the efficient storage and release of electrical energy. Highlighted areas will include coupled ionic and charge transport, electrolyte physics, theory and modeling, and novel materials and approaches.

Priority Research Directions

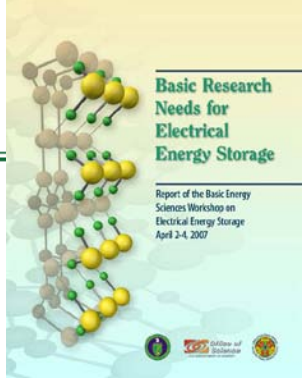
- Novel Designs and Strategies for Chemical Energy Storage
- Solid-Electrolyte Interfaces and Interphases in Chemical Energy Storage
- Capacitive Energy Storage Materials by Design
- Electrolyte Interactions in Capacitive Energy Storage
- Multifunctional Materials for Pseudocapacitors and Hybrid Devices
- Rational Materials Design Through Theory and Modeling

Cross-Cutting Science for Electrical Energy Storage

- Advances in Characterization
- Nanostructured Materials
- Innovation in Electrolytes
- Theory, Modeling and Simulation

These research priorities for electrical energy storage were echoed in the recommendations from the industry-led SciTech report in 2010

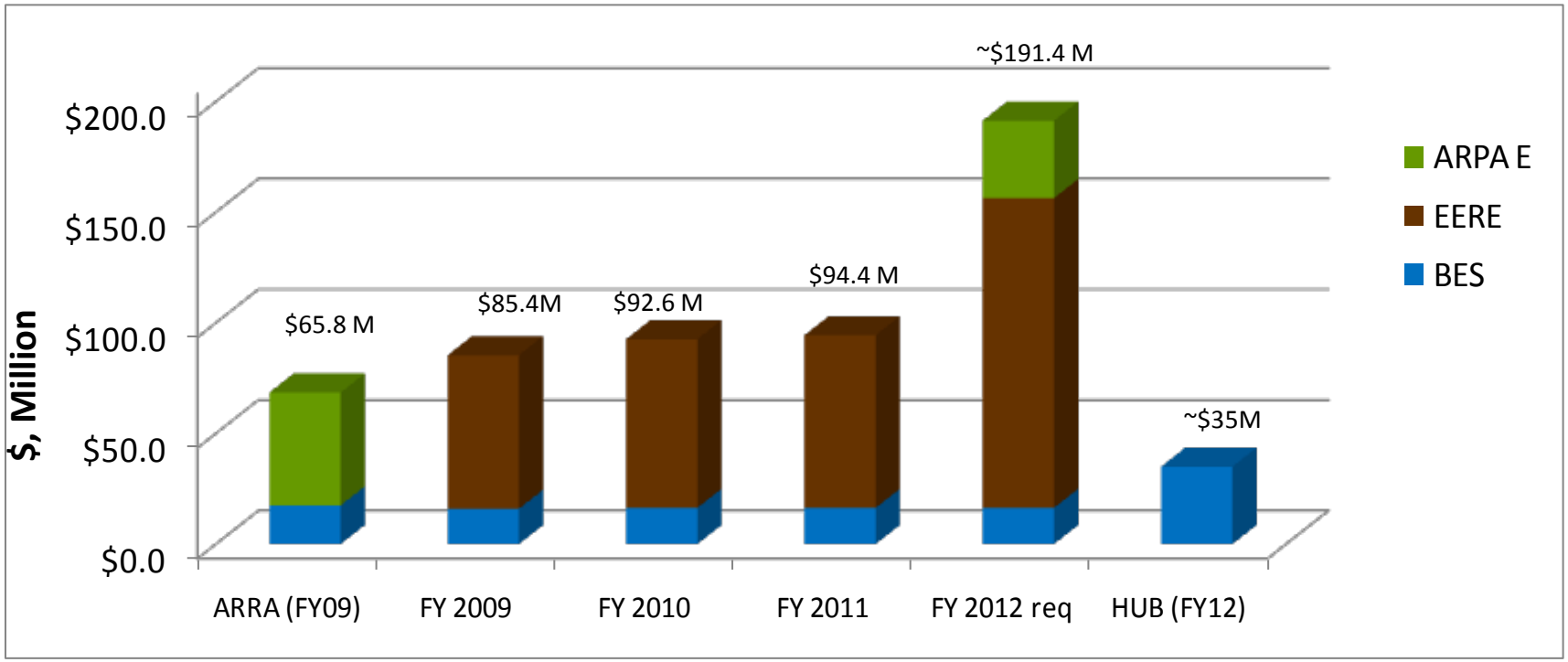
Batteries and Energy Storage: Critical Issues in Research



A Unified Research Framework for Transportation and Stationary End-use

How can we approach theoretical energy densities?	*How do we increase the rate of energy utilization and safe storage capacity?*	*Can we create a system that is close to perfectly reversible?*
- Need to know how to design and control energy transfer	- Need to improve ionic and electrical conductivity	- Need to understand interfaces and phase stability
- Need to develop novel multi-electron systems	- Need to design simple, stable nanostructures	- Need to understand system dynamics
- Need to understand fluid behavior in nanopores	- Need to understand energy transport	- Need to design new materials and structures
Increased Energy Density	Higher Power	Longer Lifetimes

Energy Storage R&D: Transportation Battery Funding



Much of the BES investment in Electrical Energy Storage research is applicable to both transportation and stationary technologies.

Energy Frontier Research Centers

Tackling Our Energy Challenges in a New Era of Science

- To engage the talents of the nation's researchers for the broad energy sciences
- To accelerate the scientific breakthroughs needed to create advanced energy technologies for the 21st century
- To pursue the fundamental understanding necessary to meet the global need for abundant, clean, and economical energy

46 centers awarded in FY 2009 ($777M over 5 years), representing 115 participating institutions in 35 states and D.C.

Pursue *collaborative* basic research topics that address both energy challenges and science grand challenges

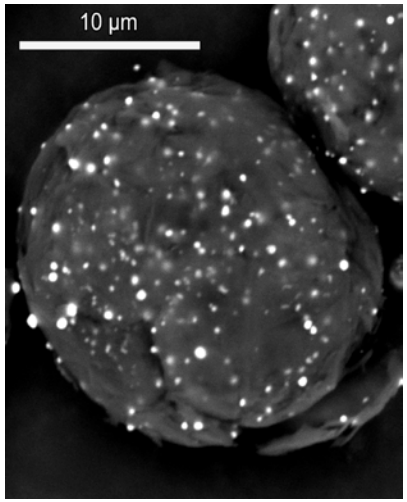
Six have a primary focus on fundamental and use-inspired research related to electrical energy storage – cross-cutting vehicle and the grid – while several others are performing underpinning science in this area

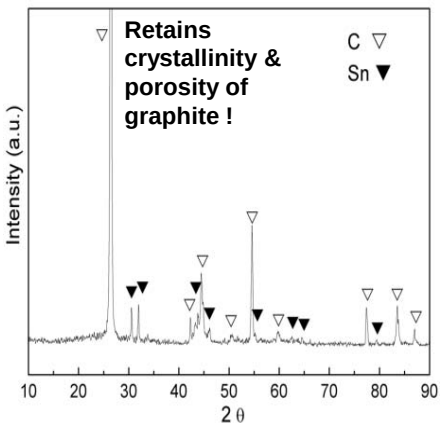
Energy Storage Research Topics in BES: Core Program and EFRCs

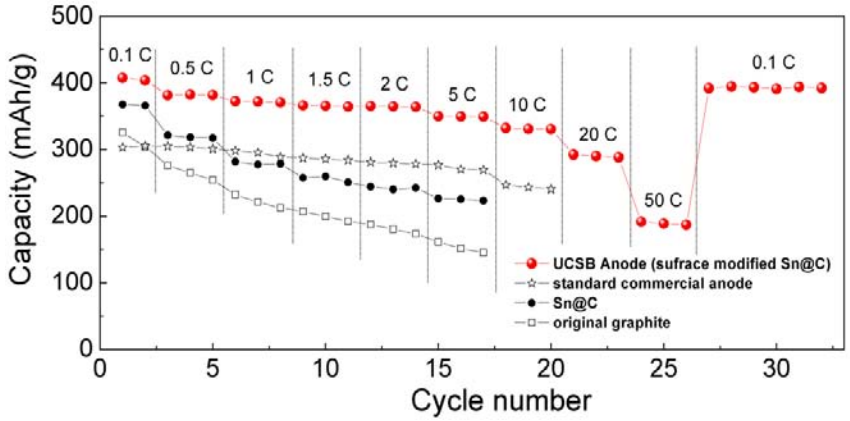
- Development of new in-situ measurement techniques
- Understanding electrolyte chemistry and behavior
- New materials for supercapacitors
- Novel materials and structures for electrode materials
- Understanding the Solid-Electrolyte Interphase (SEI) layer
- Influence of nanostructuring on behavior
- Synthesis and processing techniques including bio-inspired approaches
- Structural evolution and degradation during cycling

Selected Scientific Highlights from Recent BES-sponsored Research underpinning Electrical Energy Storage

Bioinspired Catalytic Fabrication of Tin-in-Graphite Anode for High Power Lithium-Ion Batteries





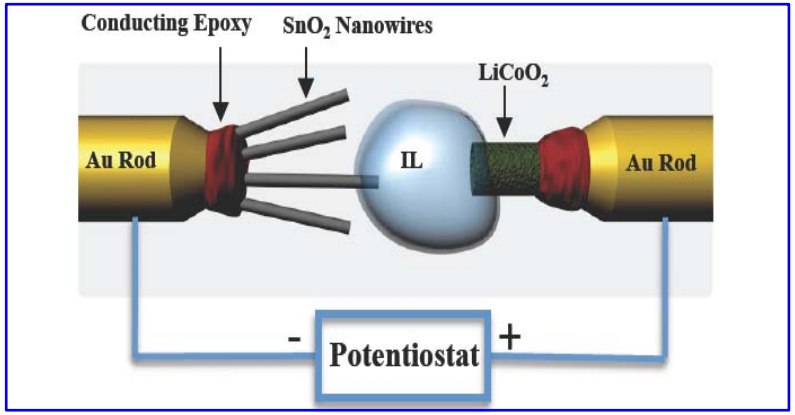


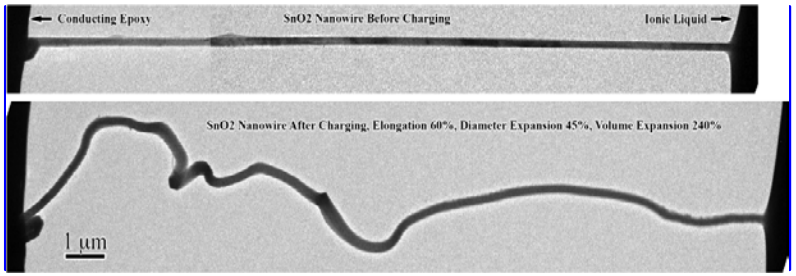
- Bio-inspired low-temperature kinetically controlled synthesis grows highly dispersed 200-500 nm Sn nanoparticles *in situ* in graphite
- Back-scattered electron image and compositional mapping show uniform dispersion of Sn throughout the graphite matrix.
- Provides high electrical capacity of the metal while the compliant graphite "breathes" to accommodate swelling and shrinking of the tin with entry and exit of Li^+ during each charge-discharge cycle
- Electrochemical measurements demonstrate that composite with Sn content of 15 wt% has a reversible capacity of 450 mAh g^{-1} with excellent retention over multiple cycles

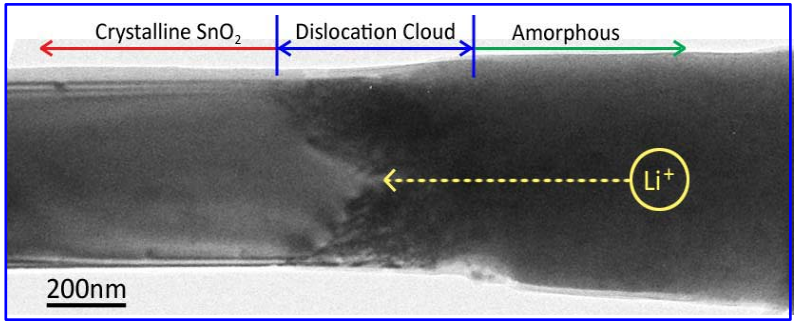
Hong-Li Zhang and Daniel E. Morse, *J. Mater. Chem*. 2009, *19*, 9006-9011

Battery in a Microscope: In-Situ Studies Showing Lithiation of SnO_2

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







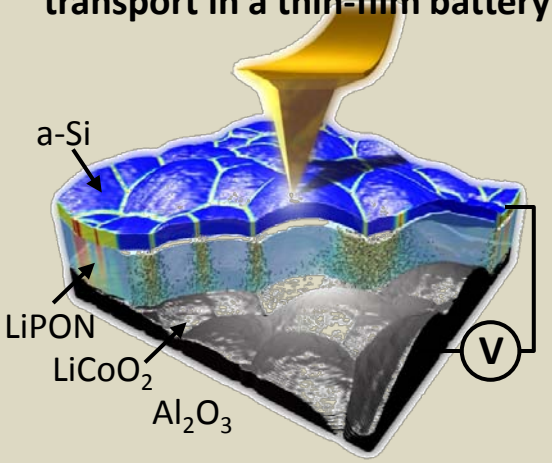
Jian Yu Huang, et al., Science 330, 1515 (2010)

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

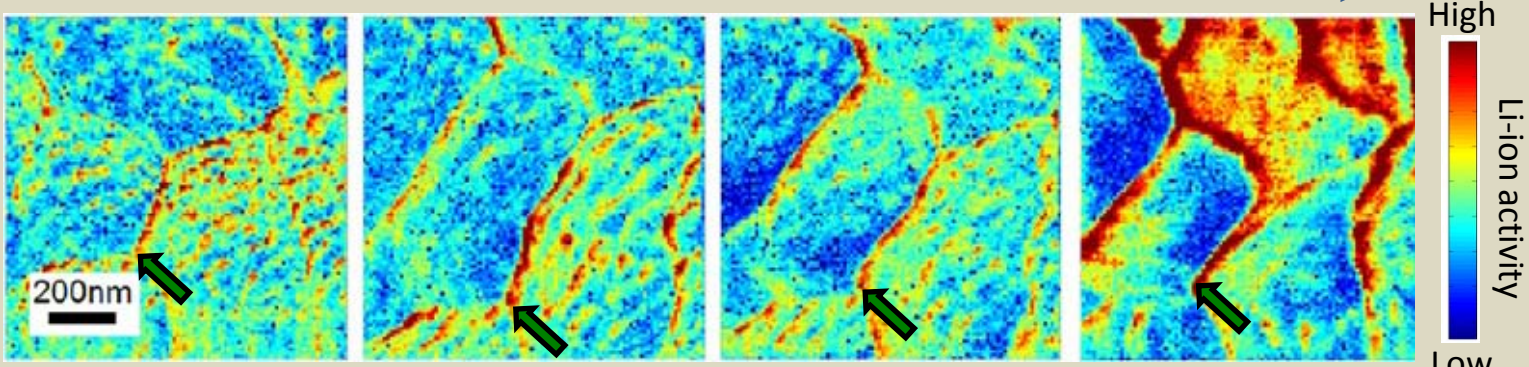
EFRC Research Demonstrates Real Space Mapping of Lithium-Ion Transport in Anodes with Nanometer Resolution

- Understanding ionic flow on a local scale is key to improving battery technologies
- Atomic force microscopy detects local volume changes in heterostructures due to ionic flow induced by tip biasing
  - Probes lithium-ion transport by high frequency biasing
- Lithium-ion flow is correlated with the structure of electrodes and interfaces
- Performed by Fluid Interface Reactions, Structures and Transport (FIRST) EFRC led by Oak Ridge National Laboratory

Atomic Force Microscopy characterizes the local lithium-ion transport in a thin-film battery



Change in Li-ion kinetics in the Si anode with increasing charging state

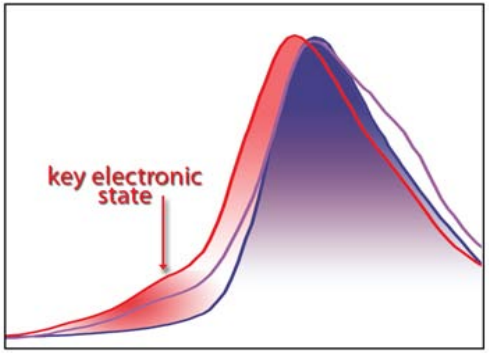


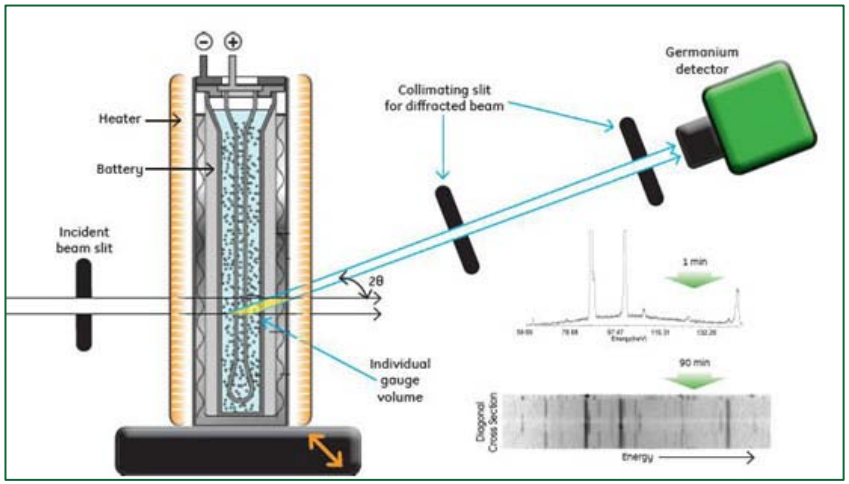
N. Balke et al, Nano Letters 10, 3420-3425 (2010).

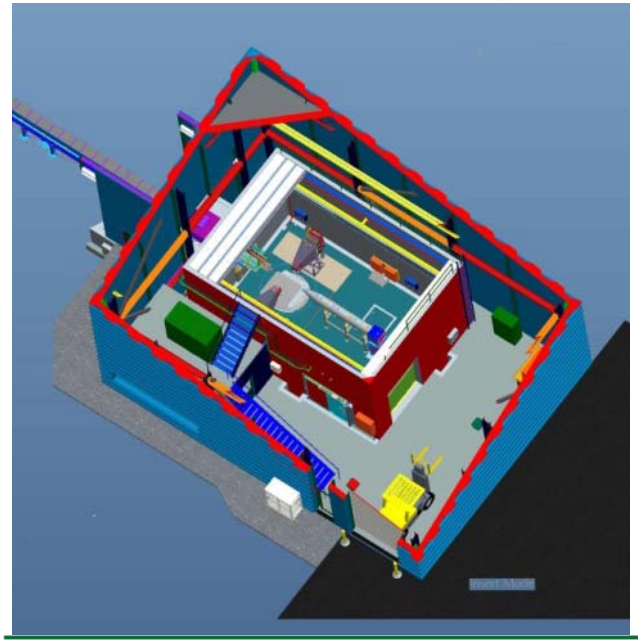
The a-Si anode surface roughness induces localized Li-ion transport which is enhanced with increasing battery charging.

BES User Facilities Developing New Capabilities for Electrical Energy Storage Research

New techniques and facilities are being developed at high-brightness light sources to measure dynamic chemical changes during battery cell operation and measure electronic states in new electrode materials.



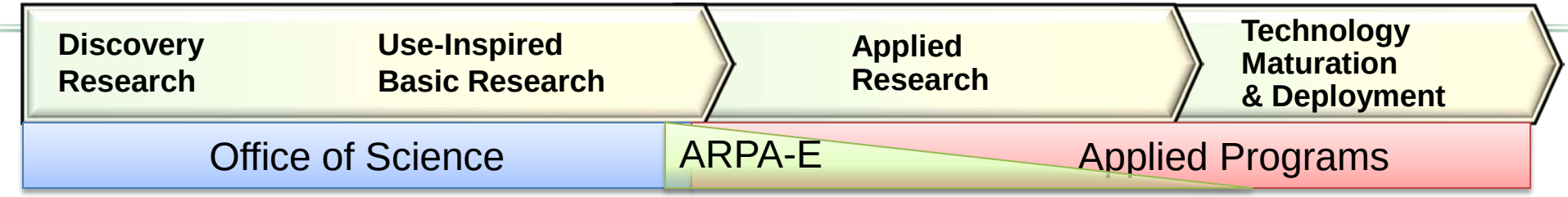




Neutron scattering facilities are developing large-scale end stations such as VULCAN that are being utilized to measure strains developed in batteries during repeated cycling, providing insight into operation and degradation.

In addition, synthesis and characterization capabilities relevant to energy storage are found at the BES Nanoscience Centers (see prior slides) and the Electron Microscopy Centers

R&D Continuum for Electrical Energy Storage



BES

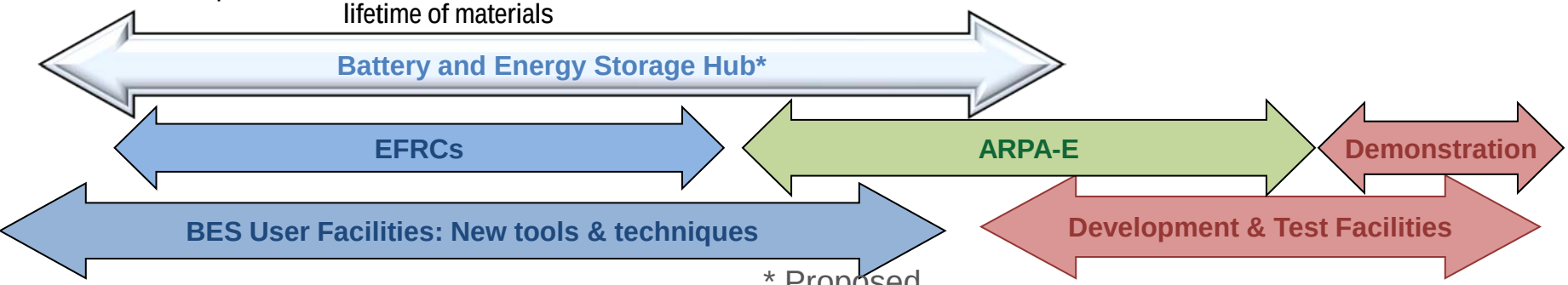
- Understand and predict interfacial charge transfer and multi-body effects
- Predict and control dynamics of phase transitions
- Control of chemistry and its dynamics at electrified interfaces
- Physicochemical consequences of nano-dimensions
- Fundamentals of solvation dynamics and ionic transport
- Retrosynthetic approaches to high performance new materials
- Design of new materials capable of multi-electron storage per redox center
- Understand design criteria for electrolytes that enable higher voltages
- Tailor nanoscale electrode architectures for optimal transport
- Novel chemistries for scavenging impurities and self-healing
- Generation of knowledge and computational and experimental tools to predict properties, performance evolution, and lifetime of materials

ARPA-E

- Quick scale-up feasibility tests of demonstrated new-generation battery technology concepts
- Rapid development of new technology concepts—demonstration within 1-2 years

EERE/OE: Significant focus on batteries and capacitors for vehicle and grid applications

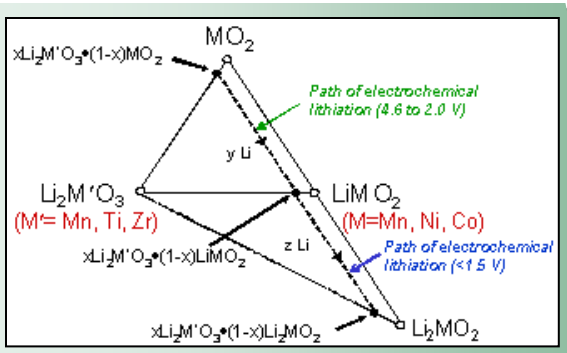
- Development of full battery systems and advanced materials for those systems
- Systems analysis which includes thermal analysis and simulation, various simulations to determine battery requirements, life modeling, and recycling studies
- Research, development, and engineering of higher energy advanced materials and cell chemistries that simultaneously address the life, performance, abuse tolerance, and cost issues.
- Deployment of full-scale grid storage systems



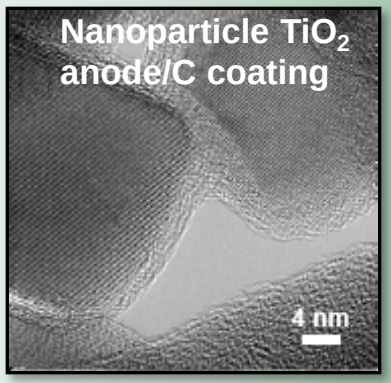
* Proposed

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

Basic Science



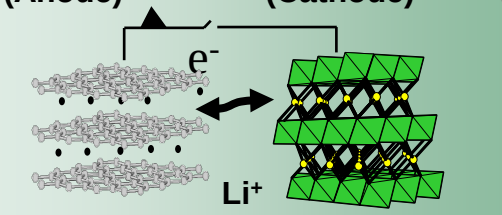
Discovered new composite structures for stable, high-capacity cathodes



EFRC research

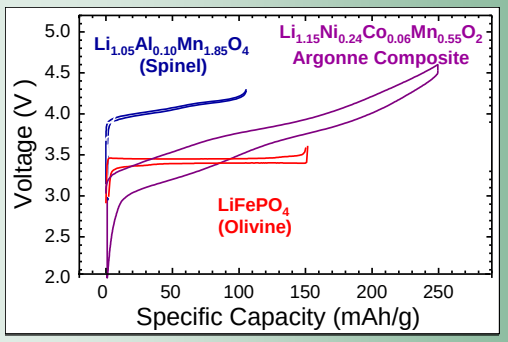
Tailored electrode-electrolyte interface using nanotechnology

Applied R&D



Created high energy Li-ion cells…

…with double cathode capacity, enhanced stability

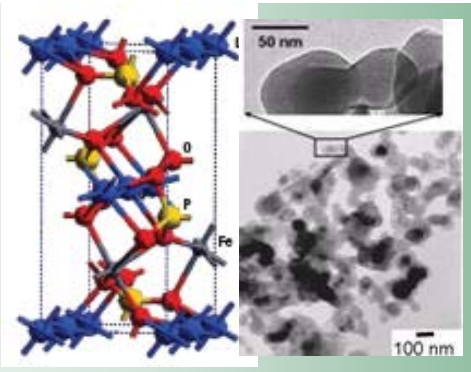


Manufacturing/ Commercialization

Licenses to materials and cell manufacturers and automobile companies

High Impact Basic Research: Nanotechnology Approach Leads to Commercial Batteries

Basic Science



$LiFePO_4$ structural model and nanostructure

- Research at MIT over a decade ago led to the discovery that drastically refining the structure of ceramics enhanced their conductivity (DOE Office of Science)
- Minor chemical additions to the fine-grained $LiFePO_4$ further increased the conductivity by eight orders of magnitude

Applied R&D

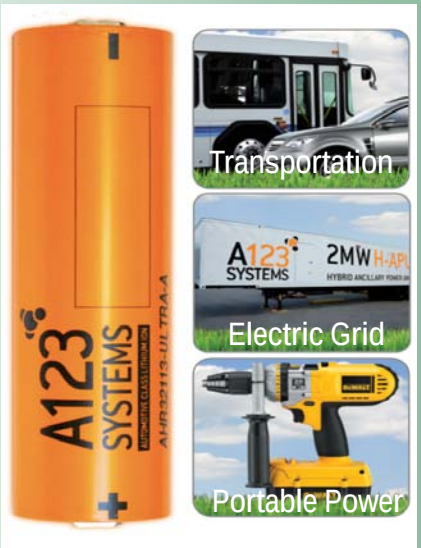
Formation of A123 Start-up

DOE Small Business Innovation Research (SBIR)

Enabled development of an A123 lithium-ion battery that

- Improved battery life by up to 10 times compared to other Li batteries
- Has more than twice the power density of high power NiCd and NiMH batteries
- Operates over a wide temperature range, from -30 to >60°C
- Charges to more than 90% capacity within 5 minutes

Manufacturing/ Commercialization



Today - A123Systems' batteries have reached the commercial marketplace in power tools, hybrid and plug-in hybrid electric vehicles, and grid applications. A recent DOE-Vehicle Technologies grant paved the way for what is now the largest lithium ion automotive battery plant in North America.

More information about BES can be found at
http://science.energy.gov/bes/