U.S. DEPARTMENT OF ENERGY | Office of Science

BES Energy Storage Research

2013 Vehicle Technologies Annual Merit Review

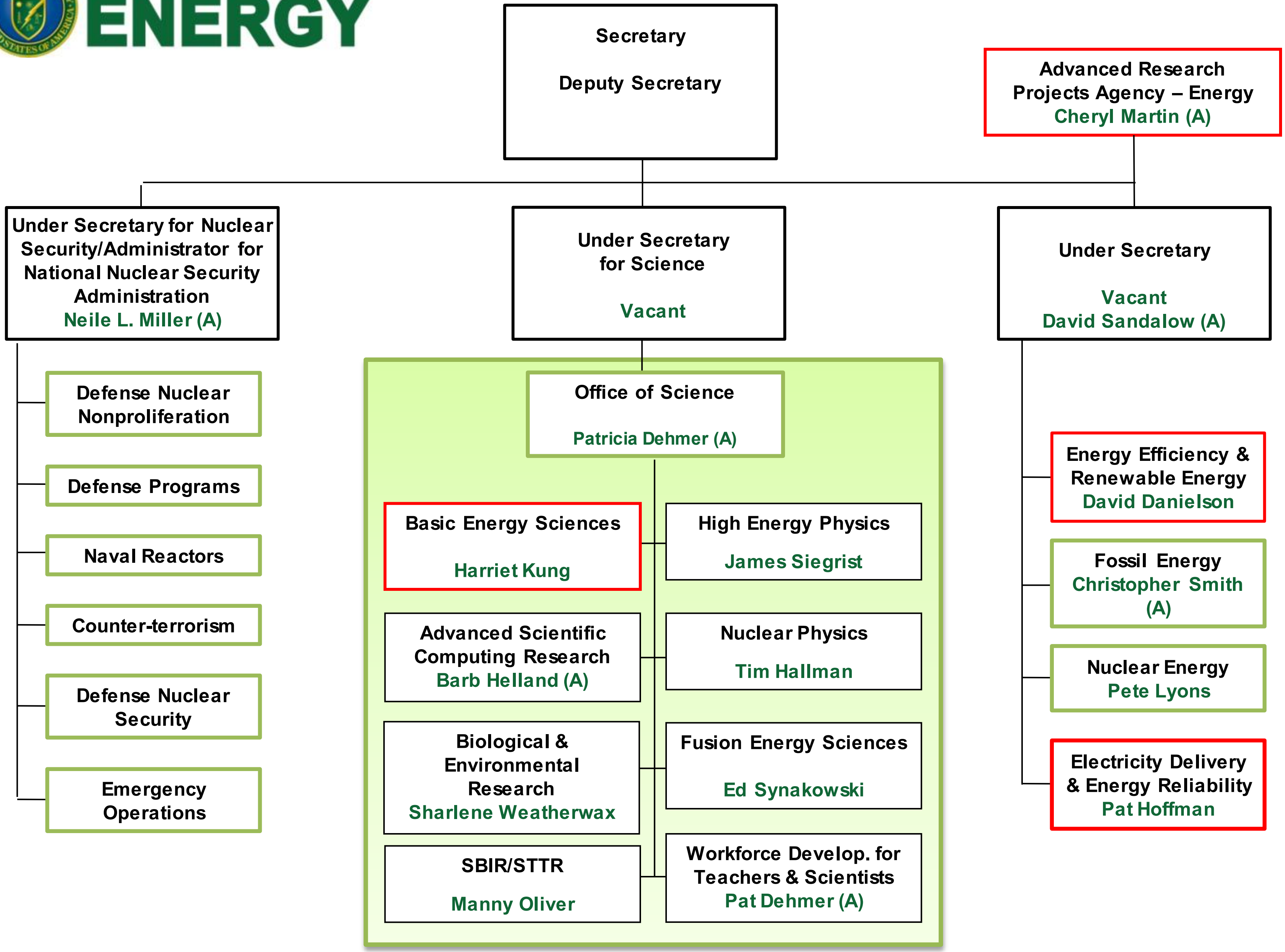
May 14, 2013

John Vetrano

Materials Sciences and Engineering Division

Office of Basic Energy Sciences

U.S. DEPARTMENT OF ENERGY



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

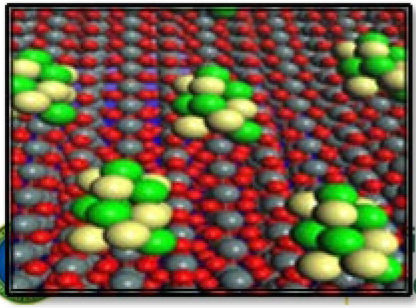
Chemical sciences, geosciences, and energy biosciences—exploring the fundamental aspects of chemical reactivity and energy transduction over wide ranges of scale and complexity and their applications to energy technologies

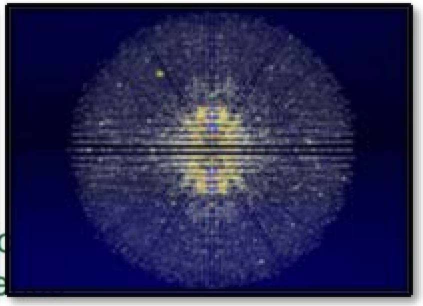
Supporting:

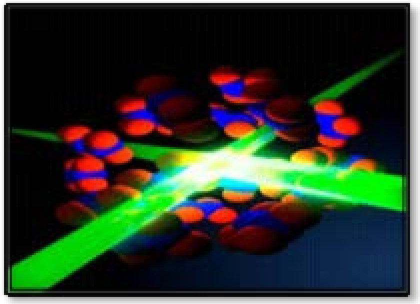
- 46 Energy Frontier Research Centers
- Two Hubs: Solar Fuels and Batteries
- The largest collection of facilities for electron, x-ray, and neutron scattering in the world

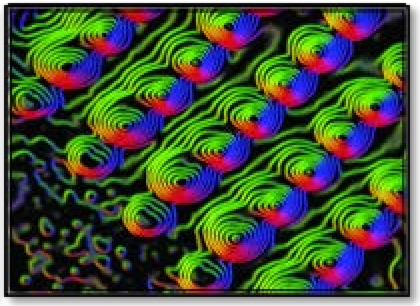
The Scientific Challenges:

- 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









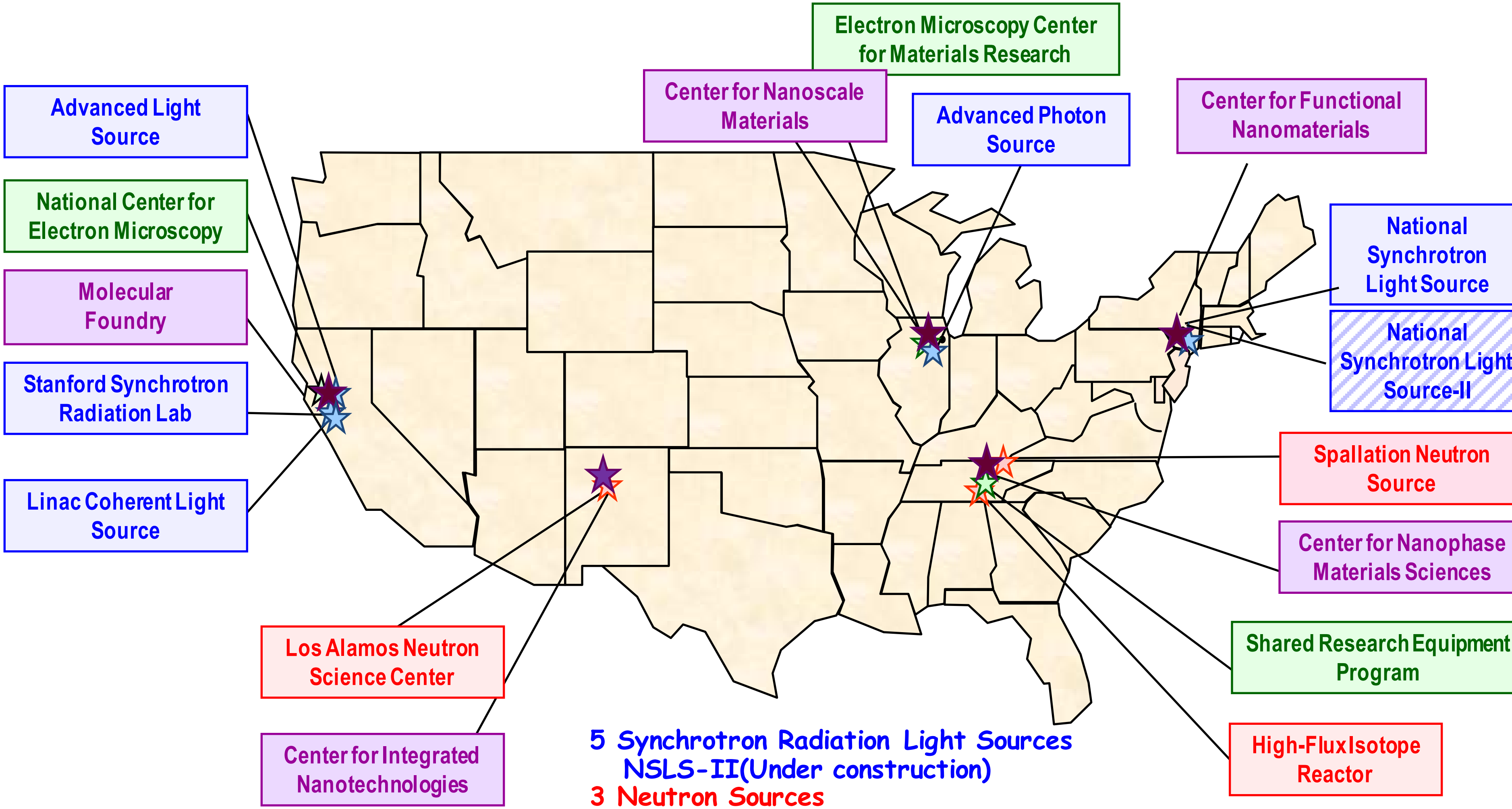
Office of Basic Energy Sciences

Office of Basic Energy Sciences
Harriet Kung, Director

- **Materials Sciences and Engineering Division**
  - Materials Discovery, Design and Synthesis
  - Condensed Matter and Materials Physics
  - Scattering and Instrumentation Sciences
- **Scientific User Facilities Division**
  - X-Ray and Neutron Scattering Facilities
  - Nanoscience and Electron Microscopy Centers
- **Chemical Sciences, Geosciences and Biosciences Division**
  - Fundamental Interactions
  - Photochemistry and Biochemistry
  - Chemical Transformations

Research grouped by scientific topics -- not by specific energy technologies

BES Scientific User Facilities: Resources for Materials Research

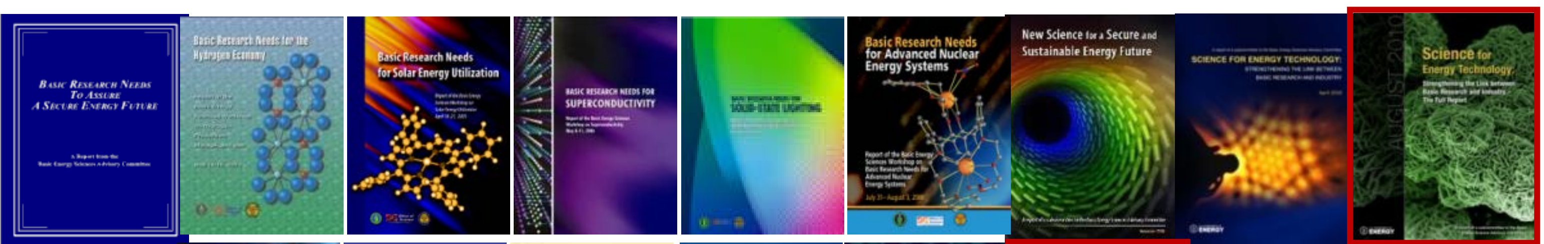


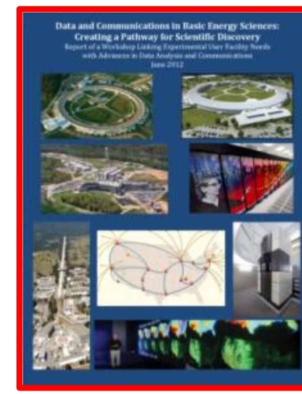
5 Synchrotron Radiation Light Sources
NSLS-II (Under construction)
3 Neutron Sources
3 Electron Beam Microcharacterization Centers
5 Nanoscale Science Research Centers

BES Strategic Planning Activities

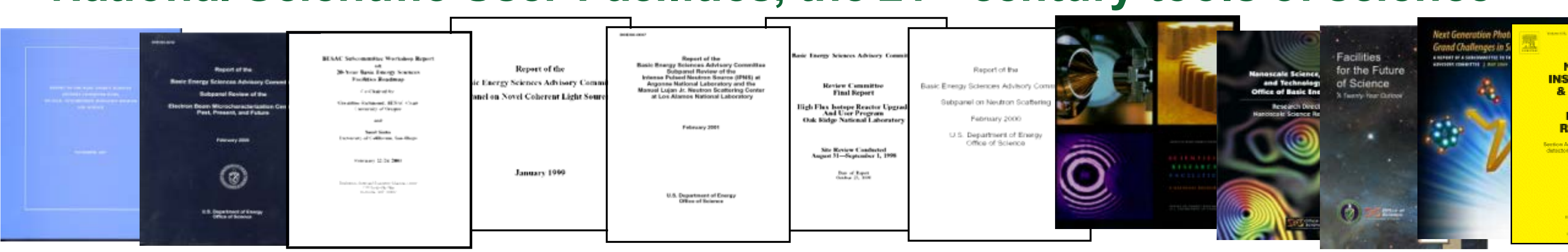
- Science for Discovery

- Science for National Needs





- National Scientific User Facilities, the 21st century tools of science



Detector R&D

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

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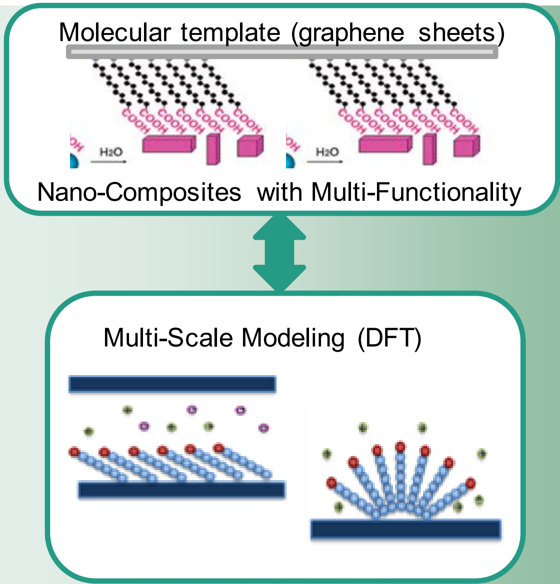
* ARPA-E: targets technology gaps, high-risk concepts, aggressive delivery times

Understanding of Self-Assembly for Multifunctional Materials Synthesis leads to Enhanced Batteries

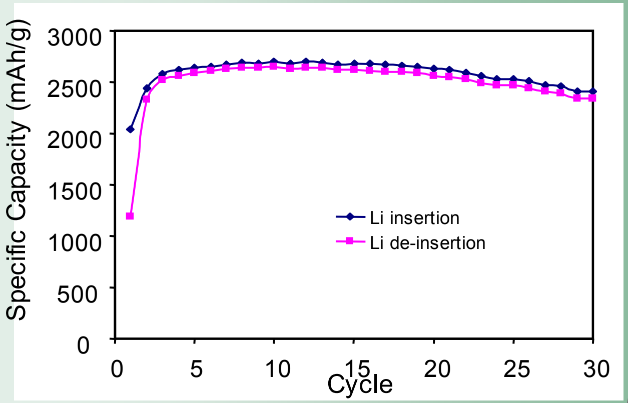
Basic Science



A systematic approach to the surfactant templated self-assembly process brought forth a basic understanding of interfacial interactions allowing the creation of 3D integrated hybrid nano-structures

Applied R&D

Surfactant-mediated growth was utilized to incorporate porous Si between graphene sheets. These sheets buffer the volume changes in Si during charge/discharge cycles in a Li-ion battery, leading to high capacity and cycle stability.



Manufacturing/ Commercialization

Vorbeck, in partnership with the Pacific Northwest National Labs (PNNL) and Princeton University, is working to commercialize lithium batteries incorporating graphene technology. This innovation would realize major improvements in the battery performance, enabling faster-charging, higher powered batteries for transportation and consumer electronics.

PRINCETON UNIVERSITY

Pacific Northwest NATIONAL LABORATORY

Vorbeck Materials

BES : Science for Discovery & National Needs

Three Research Modalities

Increasing progression of scientific scope and level of effort

- **Core Research (Grant and National Laboratory)**

  Support single investigator and small group projects to pursue their specific research interests. Includes Early Career Awards (5-year, non-renewable individual awards).

- **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 (2 in BES)**

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

BES Core Research Program

- **All research funded at national laboratories, universities, and other institutions, including facility construction and operation, is awarded through a peer-reviewed, merit-based process.**
- **White papers and proposals are considered throughout the year (Annually released, open FOA)**
- About 1/3 of DOE Office of Science research funding goes to support grants at more than 300 colleges and universities nationwide
- The Small Business Innovative Research (SBIR) Program provides funding for commercial-driven research activities
- The DOE EPSCoR program funds research in states with below average research funding
- BES User Facilities provide resources for research
  - ~15,000 users of BES scientific facilities a year
  - No cost to users, research must be published
  - Time and access are awarded through competitive review

BES Energy Frontier Research Centers: Opportunities for Collaboration on Energy Use-Inspired Research

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 representing 102 participating institutions in 36 states and D.C. Funding level for each Center is $2M - $5M/yr for five-years.

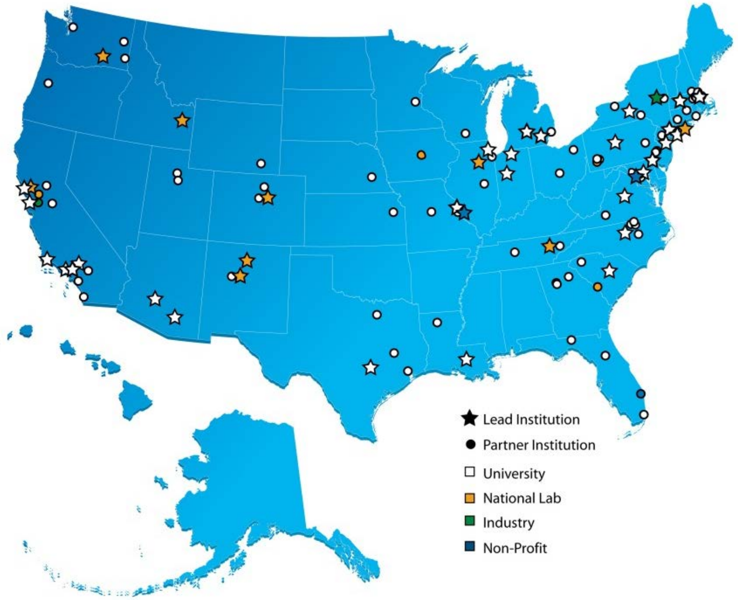
Pursue *collaborative* basic research that addresses both energy challenges and science grand challenges in areas such as:

- Solar Energy Utilization
- Combustion
- Bio-Fuels
- Catalysis
- Energy Storage
- Solid State Lighting
- Geosciences for Energy Applications
- Superconductivity
- Advanced Nuclear Energy Systems
- Materials Under Extreme Environments
- Hydrogen

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

Energy Frontier Research Centers

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

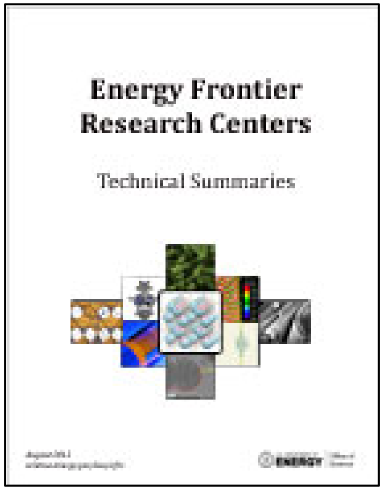


Participants:

- **46** EFRCs in **35** States + Washington D.C.
- ~**850** senior investigators and ~**2,000** students, postdoctoral fellows, and technical staff at ~**115** institutions
- > **250** scientific advisory board members from **13** countries and > **40** companies

Progress to-date (~3.5 years funding):

- >**3,400** peer-reviewed papers including >**110** publications in *Science* and *Nature*
- **18** PECASE and **11** DOE Early Career Awards
- > **200** patent/patent applications, plus an additional >**60** invention disclosures, and at least **30** licenses
- at least **60** companies have benefited from EFRC research
- EFRC students and staff now work in : > **195** university faculty and staff positions; > **290** industrial positions; > **115** national labs, government, and non-profit positions



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

BES EFRCs: Engaging the talents of the nation's researchers for the broad energy sciences

Pursuing *collaborative* basic research that addresses both energy challenges and science grand challenges in areas such as:

- Solar Energy Utilization
- Combustion
- Bio-Fuels
- Catalysis
- **Energy Storage** (includes ↓)
- Solid State Lighting
- Geosciences for Energy Applications
- Superconductivity
- Advanced Nuclear Energy Systems
- Materials Under Extreme Environments
- Hydrogen

Center for Electrical Energy Storage (CEES)
Argonne National Laboratory (M. Thackeray)

Center for Electrocatalysis, Transport Phenomena, & Materials for Innovative Energy Storage (CETM)
GE Global Research (G. Soloveichik)

Nanostructures for Electrical Energy Storage (NEES)
University of Maryland (G. Rubloff)

Northeast Center for Chemical Energy Storage (NECCES)
Stony Brook University (S. Whittingham)

Energy Materials Center at Cornell (emc^2)
Cornell University (H. Abruña)

Heterogeneous Functional Materials Center (HeteroFoaM)
University of South Carolina (K. Reifsnider)

BES EFRC Research in Energy Storage at a glance

Snapshot of EFRC Research in Energy Storage by keywords:

Basic Research Needs:	Electrical Energy Storage
Grand Challenges:	Controlling matter at the level of electrons Design/synthesis new material with tailored properties Characterize and control matter far from equilibrium
Science Topics:	Fundamental processes in batteries and fuel cells Electrode and electrolyte materials Membranes and selective transport of ions Electron transport and charge transfer Interfacial transport and chemistry Material morphology and dimensionality (1D, 2D, and 3D) Defects and material heterogeneity Nanostructured materials and nanocomposites
Experimental/ Theoretical Development	*In-situ* electron and scanning probe microscopy X-ray diffraction and scattering techniques Interfacial/surface characterization and modeling Molecular dynamics (MD) modeling and simulation Density functional theory (DFT)

DOE Energy Innovation Hubs: Multidisciplinary Research

Hubs funded in FY 2010:

- Fuels from Sunlight (SC-BES) – Joint Center for Artificial Photosynthesis (JCAP) – Caltech and LBNL
- Energy Efficient Building Systems Design (EERE) – Penn State
- Modeling and Simulation for Nuclear Fuel Cycles and Systems (NE) – ORNL

Recently Announced:

- Batteries and Energy Storage (SC-BES) – Joint Center for Energy Storage Research - ANL
- Critical Materials (EERE) – Critical Materials Institute - Ames

Each Hub has a world-class, multi-disciplinary, and highly collaborative research, development and deployment team. Funding level is $20M - $25M/yr over a five-year period

Strong scientific leadership located at the primary location of the Hub

- Clear organization and management plan for achieving the HUB goal
- "Infuses" a culture of empowered central research management

JCESR

Joint Center for Energy Storage Research

George Crabtree | JCESR Director

JCESR Impact

ACHIEVING GOALS FOR LASTING LEGACIES

TRANSPORTATION

$100/kWh

400 Wh/kg **400** Wh/L

800 W/kg **800** W/L

1000 cycles

80% DoD C/5

15yr calendar life

EUCAR

GRID

$100/kWh

95% round-trip efficiency at C/5 rate

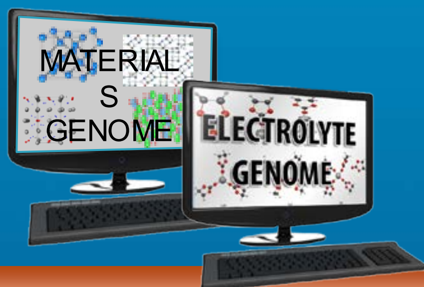
7000 cycles C/5

20yr calendar life

Safety equivalent to a natural gas turbine

- Transformational goals: 5-5-5
  - 5 times greater energy density
  - 1/5 cost
  - within 5 years
- Legacies
  - Pre-commercial prototypes for grid and transportation
  - Library of fundamental knowledge
    - Atomic and molecular understanding of battery phenomena
  - New paradigm of battery development
    - Science-based rational design
    - Systems-centric
    - End-to-end integration

The JCESR Paradigm: Beyond Lithium Ion



CROSSCUTTING SCIENCE

Multivalent Intercalation

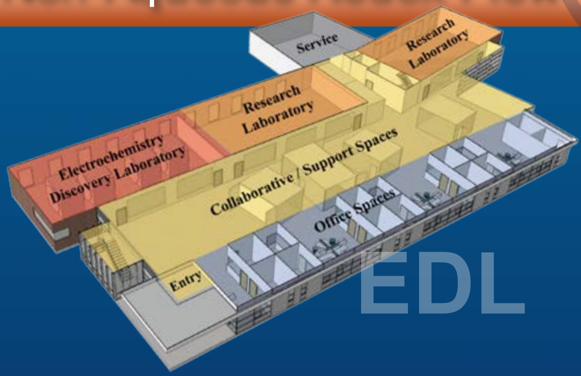
Chemical Transformation

Non-Aqueous Redox Flow

Systems Analysis and Translation

Cell Design and Prototyping

Commercial Deployment



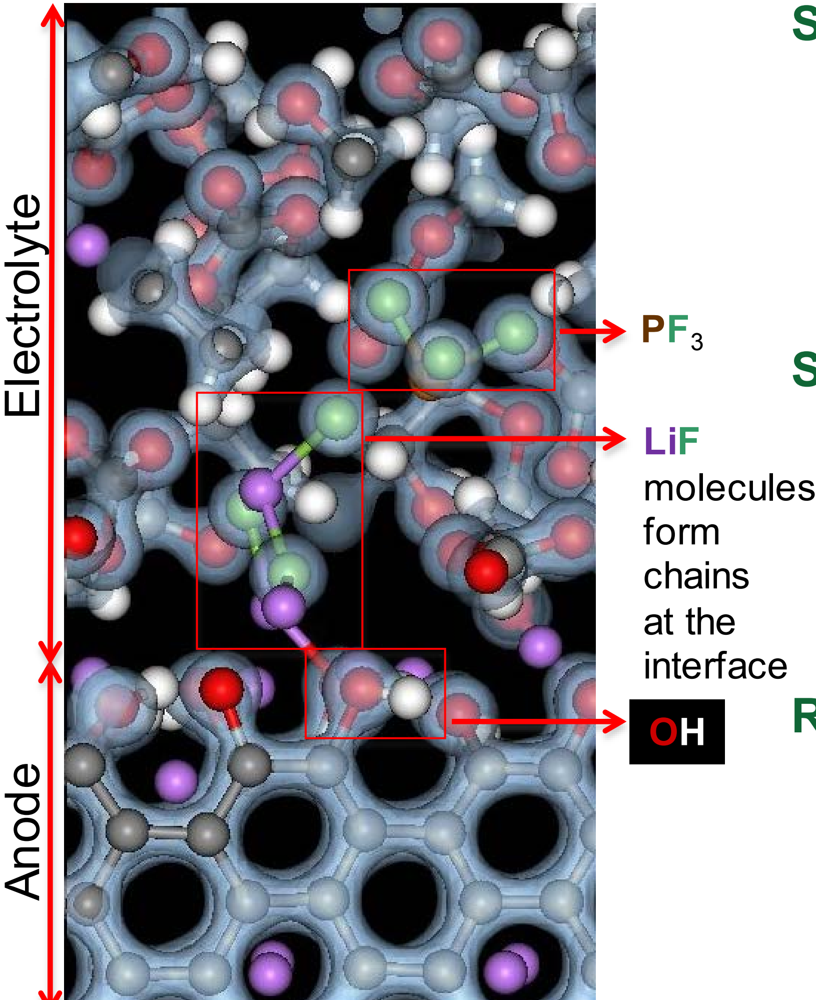
EDL

TECHNO-ECONOMIC MODELING

DISTINGUISHING TOOLS

END-TO-END INTEGRATION

Ab Initio Simulation of Solid-Electrolyte Interphase (SEI) Formation on Li-Ion Battery Anode Surface



Scientific Achievement

Spontaneous reduction of a Li-ion battery electrolyte salt ($LiPF_6$) has been detailed for the first time, elucidating formation of passivating LiF agglomerates and other species forming the incipient SEI on a graphitic anode surface

Significance and Impact

Salt ($LiPF_6$) reduction and LiF agglomeration explains previous experiments finding LiF as the main SEI component. This opens the possibility of making an 'artificial SEI' with amorphous LiF thin films, creating a stable SEI with high Li-ion transfer rates

Research Details

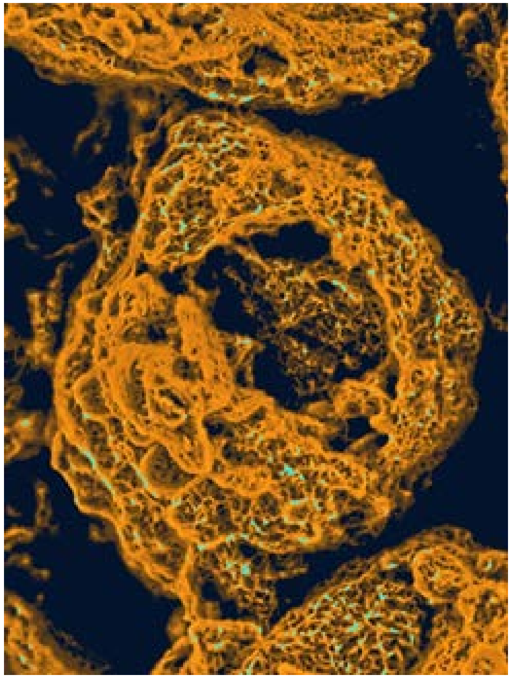
–An *ab initio* molecular dynamics study finds that electrolyte reduction is accelerated at O/OH-terminated edges of the graphite sheets.

–$LiPF_6$ reduction produces LiF, which agglomerates at anode interface blocking further destruction of $LiPF_6$

P. Ganesh, P. R. C. Kent and De-en Jiang, *J. Phys. Chem. C*, 2012, *116*, 24476-24481.

Oak Ridge National Laboratory Research supported by the FIRST EFRC.

Graphene Produces High-Capacity Li-Air Batteries for Energy Storage



Hierarchical porous electrode made of self-assembled functionalized graphene sheets. The pores enhance the air diffusion and the defects on graphene enhance the activity.

Jie Xiao, J. Liu D Mei, X Li, W Xu, D Wang, GL Graff, WD Bennett, Z Nie, LV Saraf, IA Aksay, J Zhang *Nano Letters*, 2011, *11*, 5071-5078.

Worked was performed at Pacific Northwest National Laboratory and Princeton University

Scientific Achievement

Hierarchical graphene self-assembled on oil-water interfaces produces exceptionally high energy storage capacity electrodes due to the unique pore structure and the high number of reactive sites.

Significance and Impact

This study developed a new self-assembly approach to obtain 3D graphene architectures and verified for the first time that defects are the active site for electrochemical reactions.

Research Details

– Self-assembly approaches produce graphene electrodes with a hierarchical porous material.

– Hierarchical pore structure enhances the air flow in the electrodes and increases the surface area for the electrochemical reactions.

– Detailed electron microscopy and computer modeling prove that the defects on graphene are the reactive sites and increase the energy storage capacity of these electrodes.