U.S. DEPARTMENT OF ENERGY | Office of Science

Basic Science for Advanced Energy

Advanced Energy 2009

November 18, 2009

Linda Horton
Division of Materials Sciences and Engineering
Office of Basic Energy Sciences, Office of Science
U.S. Department of Energy

Basic Energy Sciences Mission

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

Priorities:

- Discover and design new materials and molecular assemblies with novel function, through atom-by-atom and molecule-by-molecule control
- Conceptualize, calculate, and predict processes underlying physical and chemical transformations
- Probe, understand, and control the interactions of phonons, photons, electrons, and ions with matter to direct and control energy flow in materials and chemical systems
- To foster integration of the basic research with research in the DOE technology programs and NNSA

Office of Basic Energy Sciences

Harriet Kung, Director

Wanda Smith, Administrative Specialist

BES Budget and Planning

Bob Astheimer, Senior Technical Advisor
Margie Davis, Financial Management
Vacant, Program Support Specialist

BES Operations

Rich Burrow, DOE Technical Office Coordination
Don Freeburn, DOE and Stakeholder Interactions
Robin Hayes, AAAS Fellow
Katie Perine, Program Analyst / BESAC
Ken Rivera, Laboratory Infrastructure / ES&H

Materials Sciences and Engineering Division

Linda Horton, Director

◆ Ehsan Khan, Senior Technical Advisor
Christie Ashton, Program Analyst
☆ Charnice Waters, Secretary

Materials Discovery, Design, and Synthesis

Arvind Kini
Kerry Gorey, P.A.

- Materials Chemistry — Mary Galvin, Dick Kelley
- Biomolecular Materials — Mike Markowitz
- Synthesis and Processing — Bonnie Gersten
- Tech. Coordination Program Management — John Vetrano, Vacant

Condensed Matter and Materials Physics

Jim Horwitz
Marsophia Agnant, P.A.

- Exp. Cond. Mat. Phys. — Andy Schwartz, ● Doug Finnemore, Ames, Vacant
- Theo. Cond. Mat. Phys. — Vacant, △ Arun Bansil, NEU, ■ Jim Davenport, BNL, ● Kim Ferris, PNNL
- Physical Behavior of Materials — Refik Kortan
- Mechanical Behavior and Radiation Effects — John Vetrano

Scattering and Instrumentation Sciences

Helen Kerch
Cheryl Howard, P.A

- X-ray Scattering — Lane Wilson
- Neutron Scattering — Thiyaga P. Thiyagarajan
- Electron and Scanning Probe Microscopies — Jane Zhu
- DOE EPSCoR* — Tim Fitzsimmons, ● Helen Farrell, INL

* Experimental Program to Stimulate Competitive Research

Scientific User Facilities Division

Pedro Montano, Director

Linda Cerrone, Program Support Specialist
Rocio Meneses, Program Assistant

Operations

- X-ray and Neutron Scattering Facilities — Roger Klaffky, Vacant
- NSRCs & EBMCs** — Tof Carim, ◆ Joe Horton, ORNL, Vacant
- Accelerator and Detector R&D — Eliane Lessner
- Facility Coordination, Metrics, Assessment — Van Nguyen

Construction

- Linac Coherent Light Source — Tom Brown
- NSLS II — Tom Brown
- Spallation Neutron Source Upgrades — Tom Brown
- Instrument MIEs (SING, LUSI, etc.) — ◆ John Tapia, LANL
- Advanced Light Source User Support Building — Tom Brown

** Nanoscale Science Research Centers & Electron Beam Microcharacterization Centers

Chemical Sciences, Geosciences, and Biosciences Division

Eric Rohlfing, Director

Diane Marceau, Program Analyst
Michaelene Kyler-King, Program Assistant

Fundamental Interactions

Michael Casassa
Robin Felder, P.A.

- Atomic, Molecular, and Optical Sciences — Jeff Krause
- Gas-Phase Chemical Physics — Wade Sisk, △ Larry Rahn, SNL
- Condensed-Phase and Interfacial Mol. Science — Greg Fiechtner
- Computational and Theoretical Chemistry — Mark Pederson

Photo- and Bio-Chemistry

Rich Greene

- Solar Photochemistry — Mark Spitler, ● Arthur Frank, NREL
- Photosynthetic Systems — Gail McLean
- Physical Biosciences — Robert Stack

Chemical Transformations

John Miller
Teresa Crockett, P.A.

- Catalysis Science — Paul Maupin, Raul Miranda
- Heavy Element Chemistry — Lester Morss, ● Norm Edelstein, LBNL
- Separations and Analysis — Bill Millman, △ Larry Rahn, SNL
- Geosciences — Nick Woodward
- Technology Office Coordination — Marvin Singer, Vacant

LEGEND

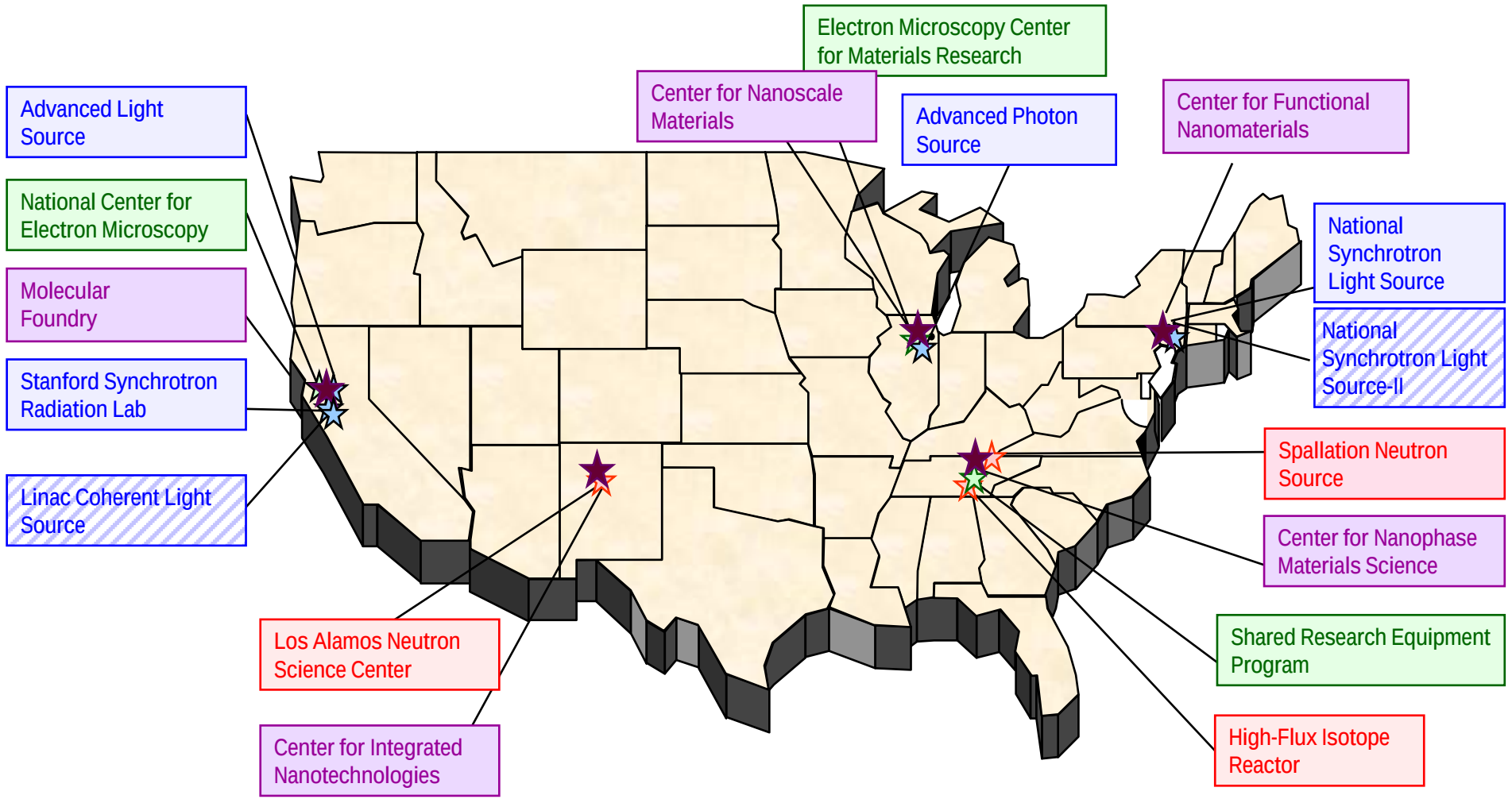
- ◆ Detailee (from DOE laboratories)
- ■ Detailee, ½ time
- ■ Detailee, ½ time, not at HQ
- ● Detailee, ¼ time, not at HQ
- ◆ On detail from SC-2, ½ time
- △ IPA (Interagency Personnel Act)
- ☆ On active military duty
- P.A. Program Assistant

November 2009

Posted 01OCT09

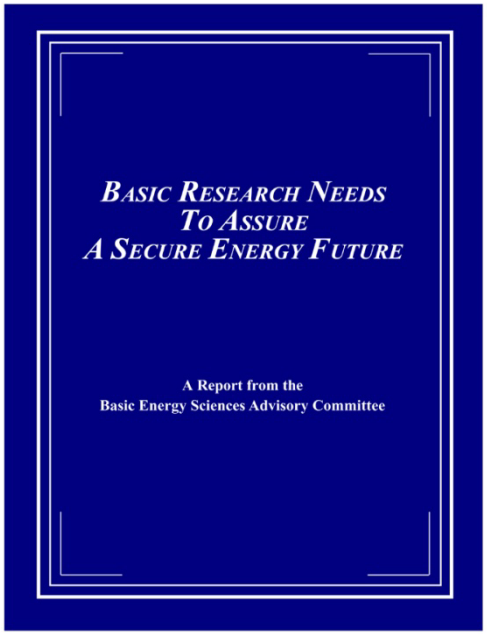
U.S. DEPARTMENT OF ENERGY

BES Scientific User Facilities: Resources for Energy Research



- 4 Synchrotron Radiation Light Sources
- Linac Coherent Light Source (Under construction)
- 3 Neutron Sources
- 3 Electron Beam Microcharacterization Centers
- 5 Nanoscale Science Research Centers

Strategic Planning
Basic Research Needs To Assure A Secure Energy Future



BESAC Basic Research Needs to Assure A Secure Energy Future Report
February 2003

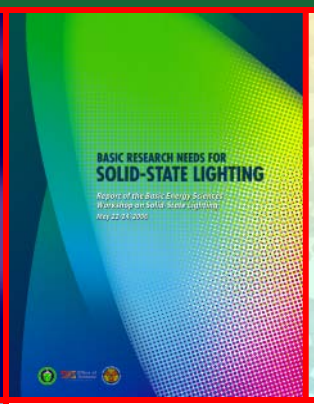
World's energy needs will more than double by 2050

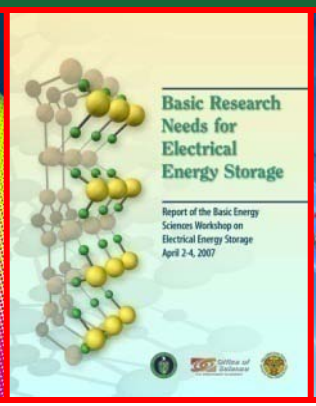
- Increasing demands for "clean" energy sources
  - Reduce atmospheric CO_2 levels
- Challenges cannot be fully met by existing technologies
- Scientific breakthroughs are required to provide reliable, economic solutions

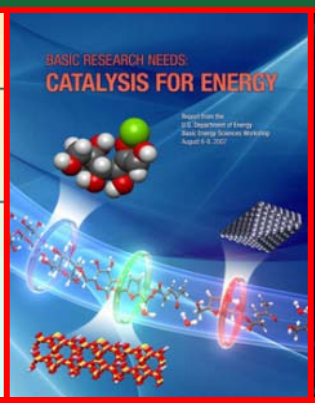
2003 Workshop and Report

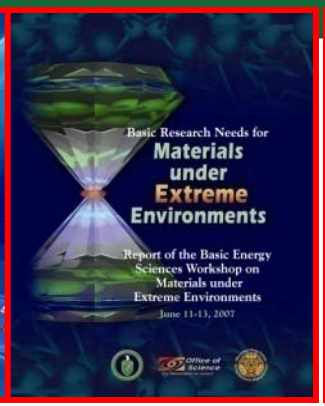
- Indentified broad, basic research directions to support the scientific advances to resolve major energy technological changes
- Series of ten follow-on *Basic Research Needs* workshops
  - >1,500 participants from universities, industry, and federal laboratories
  - In-depth analyses of scientific research that can further our Nation's most challenging energy missions

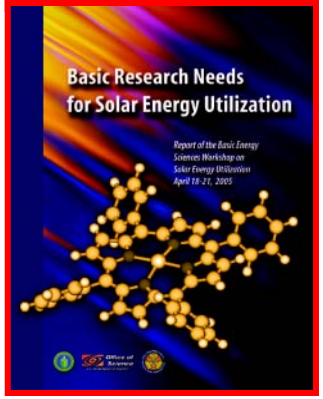
Strategies: Ten "Basic Research Needs …" Workshops



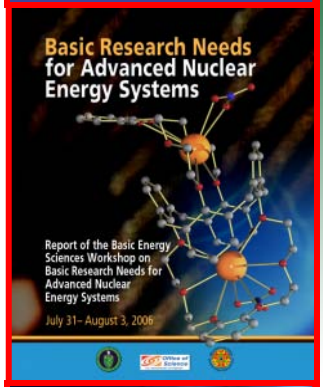


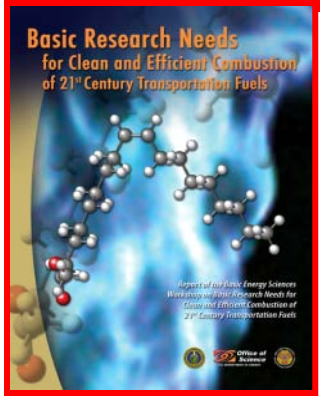






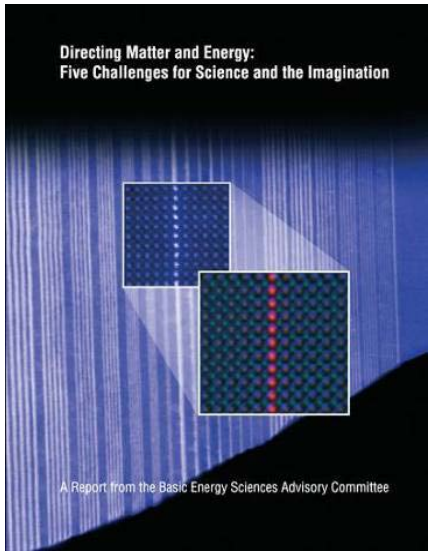
- Hydrogen Economy
- Solar Energy Utilization
- Superconductivity
- Solid State Lighting
- Advanced Nuclear Energy Systems
- Clean and Efficient Combustion of 21st Century Transportation Fuels
- Geosciences: Facilitating 21st Century Energy Systems
- Electrical Energy Storage
- Catalysis for Energy Applications
- Materials under Extreme Environments





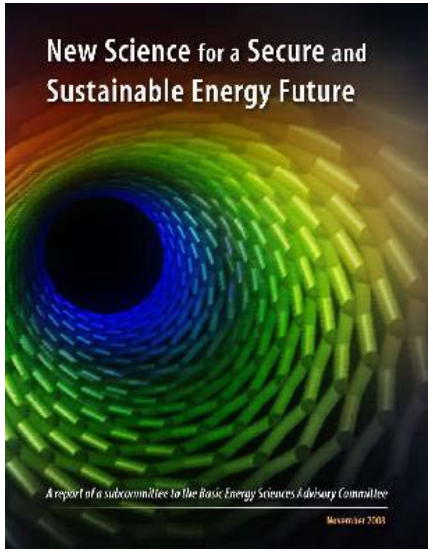
www.science.doe.gov/bes/reports/list.html

Directing Matter and Energy: Five Challenges for Science and the Imagination



- Control the quantum behavior of electrons in materials
- Synthesize, atom by atom, new forms of matter with tailored properties
- Control emergent properties that arise from the complex correlations of atomic and electronic constituents
- Synthesize man-made nanoscale objects with capabilities rivaling those of living things
- Control matter very far away from equilibrium

New Science for a Secure and Sustainable Energy Future



Goals :

- Make fuels from sunlight
- Generate electricity without carbon dioxide emissions
- Revolutionize energy efficiency and use

Recommendations:

- Work at the intersection of control science and complex functional materials
- Increase the rate of discoveries
- Establish “dream teams” of talent, equipped with forefront tools, and focused on the most pressing challenges to increase the rate of discovery
- Recruit the best talent through workforce development to inspire today’s students and young researchers to be the discoverers, inventors, and innovators of tomorrow’s energy solutions

Energy Sustainability and Control Science

Traditional Energy Materials	*Sustainable Energy Materials*
Fuels: coal, oil, gas $CH_{0.8}$, CH_2, CH_4	Diverse Functions PV, Superconductors, Photocatalysts Battery Electrodes Electrolytic Membranes
Passive Function: Combustion	Active Function: Converting Energy
Value: Commodities High Energy Content	Value: Functionality 30 year Lifetime

Greater Sustainability = Greater Complexity,
Higher Functional Control

Priority: Science and Discovery
Invest in science to achieve transformational discoveries

- **Focus on transformational science**
  - Connect basic and applied sciences
  - Double the Office of Science budget
  - Embrace a degree of risk-taking in research
  - Create an effective mechanisms to integrate university, national laboratory, and industry activities
- **Develop science and engineering talent**
  - Train the next generation of scientists and engineers
  - Attract and retain the most talented researchers
- **Collaborate universally**
  - Partner globally
  - Support the developing world
  - Build research networks across departments, government, nation and the globe

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 ($777M over 5 years), representing 102 participating institutions in 36 states and D.C.

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

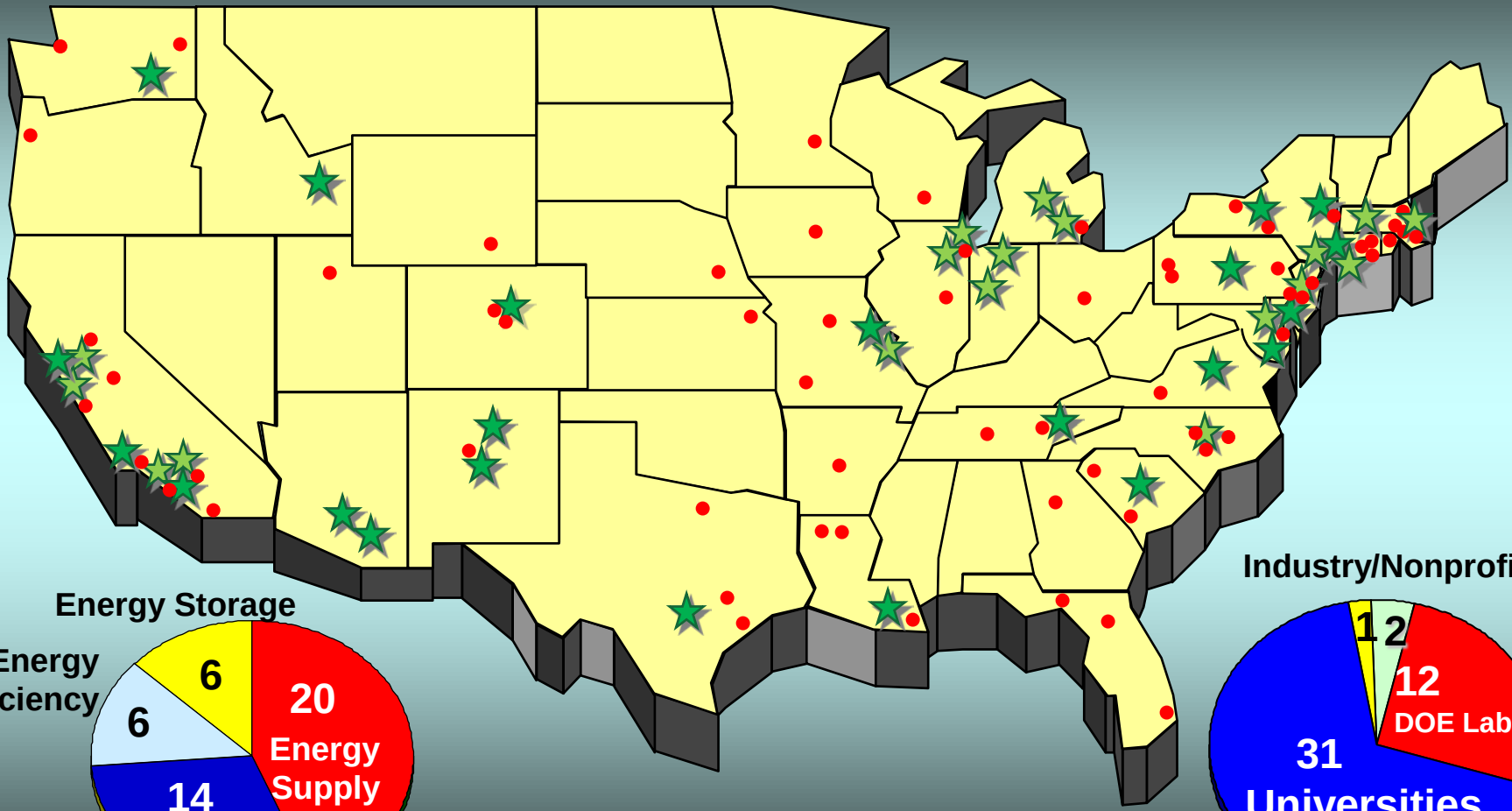
- Solar Energy Utilization
- Combustion
- Bio-Fuels
- Catalysis
- Energy Storage
- Solid State Lighting
- Geosciences for Energy Applications
- Superconductivity
- Advanced Nuclear Energy Systems
- Materials Under Extreme Environments
- Hydrogen

U.S. DEPARTMENT OF ENERGY

Energy Frontier Research Centers

46 centers awarded, representing 102 participating institutions in 36 states plus D.C

Energy Frontier Research Center Locations (★ Leads; • Participants)



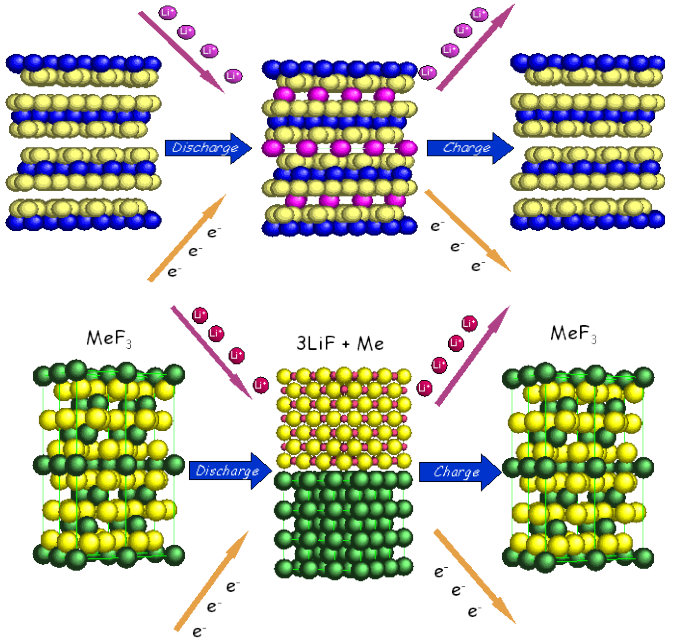
By Topical Category

By Lead Institution

Northeastern Chemical Energy Storage Center (NECESC)

Clare Grey (Stony Brook University)

Summary statement: A fundamental understanding of how key electrode reactions occur, and how they can be controlled will be developed, so as to identify critical structural and physical properties that are vital to improving battery performance; this information will be used to optimize and design new electrode materials.



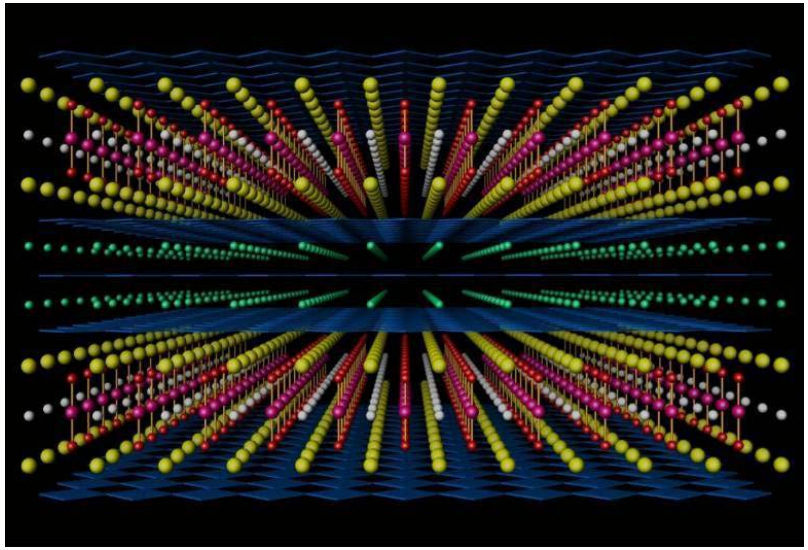
RESEARCH PLAN AND DIRECTIONS

The processes that occur in batteries are complex, spanning a wide range of time and length scales. The assembled team of experimentalists and theorists will make use of, and develop new spectroscopy, scattering, imaging and theoretical methodologies to determine how electrodes function in real time, as batteries are cycled.

Center for Emergent Superconductivity

Seamus Davis (Brookhaven National Lab)

The objectives of CES are to explore and develop higher temperature and higher critical current superconductivity with the potential for application to a superconducting power grid.



CES RESEARCH PLAN AND DIRECTIONS

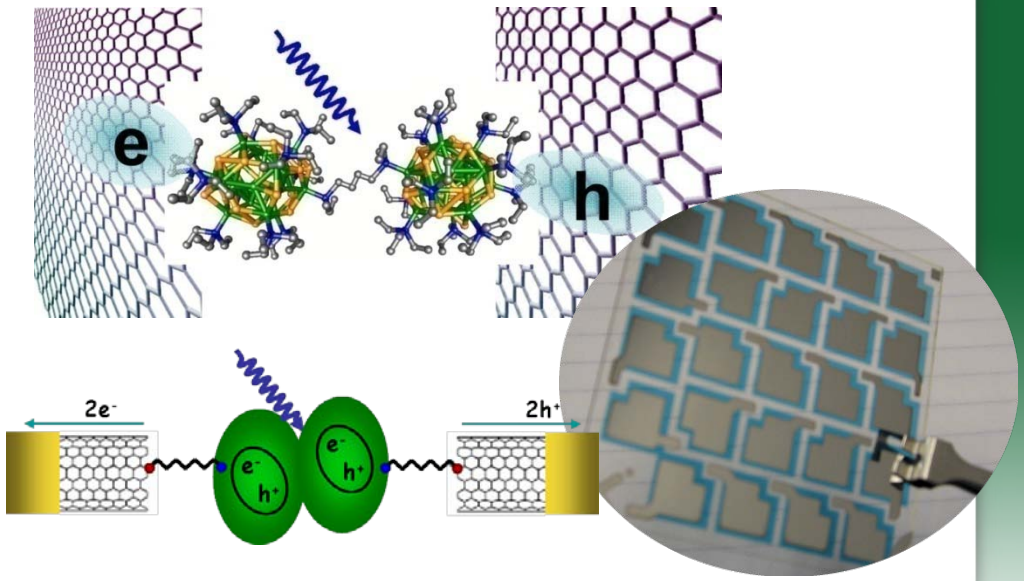
CES research will be directed towards three key areas: finding new strongly correlated superconducting materials, understanding the mechanisms leading to higher temperature superconductivity, and controlling vortex matter so as to raise the loss-less current carrying performance of these superconductors.

U.S. DEPARTMENT OF ENERGY | Office of Science
BROOKHAVEN NATIONAL LABORATORY
Argonne NATIONAL LABORATORY

Re-Defining Photovoltaic Efficiency Through Molecule Scale Control

James Yardley (Columbia University)

The Columbia EFRC will create enabling technology to re-define efficiency in nanostructured thin-film organic photovoltaic devices through fundamental understanding and through molecule-scale control of charge formation, separation, extraction, and transport.



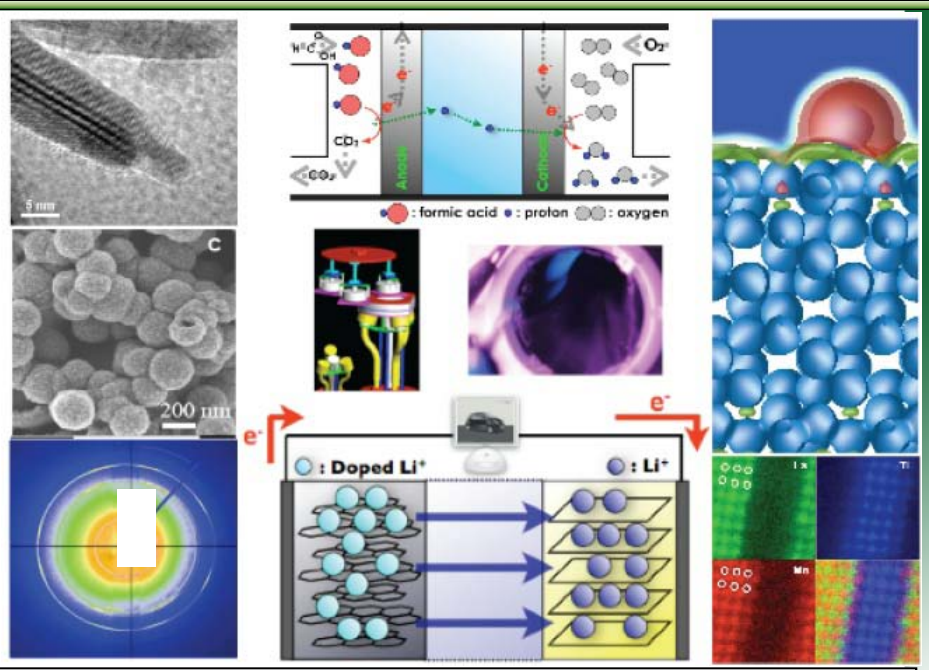
RESEARCH PLAN AND DIRECTIONS

Fundamental understanding of photo-physical and kinetic properties on the nanoscale will allow us to design systems for efficient photovoltaic generation and separation of charges. By using new conducting materials such as graphene we can transport these charges to macroscopic electrical systems, providing basis for revolutionary low cost, high efficiency devices.

U.S. DEPARTMENT OF ENERGY | Office of Science
UNIVERSITY of ARKANSAS
PURDUE

Energy Materials Center at Cornell (EMC²)
Héctor D. Abruña (Cornell University)

Summary statement: We aim to achieve a detailed understanding, via a combination of synthesis of new materials, experimental and computational approaches, of how the nature, structure, and dynamics of nanostructured interfaces affect energy generation, conversion and storage with emphasis on fuel cells and batteries.

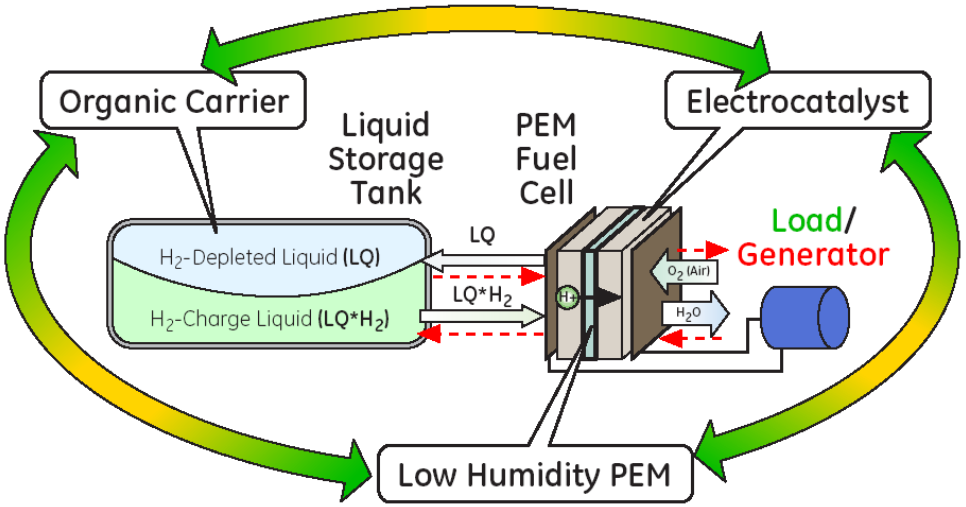


RESEARCH PLAN AND DIRECTIONS

The major challenges relate to materials performance in energy generation, conversion and storage technologies especially fuel cells and batteries. To address these, we will prepare and characterize novel nanoscale materials including ordered intermetallic phases and “atomically engineered” complex oxides. These will be characterized through novel experimental tools and computational platforms.

Center for Electrocatalysis,Transport Phenomena, and Materials for Innovative Energy Storage
Dr. Grigorii Soloveichik (GE Global Research)

Electrocatalysis, transport phenomena and membrane materials research aime to three novel components of an entirely new high-density energy storage systen combining the best properties of a fuel cell and a flow battery: organic carriers, electro(de)hydrogenation catalysts, and compatible PEM



RESEARCH PLAN AND DIRECTIONS

Challenges: Effective electrocatalysts for (de)hydrogenation of organic carriers
Transport of protons and electrons
Compatibility of cell components

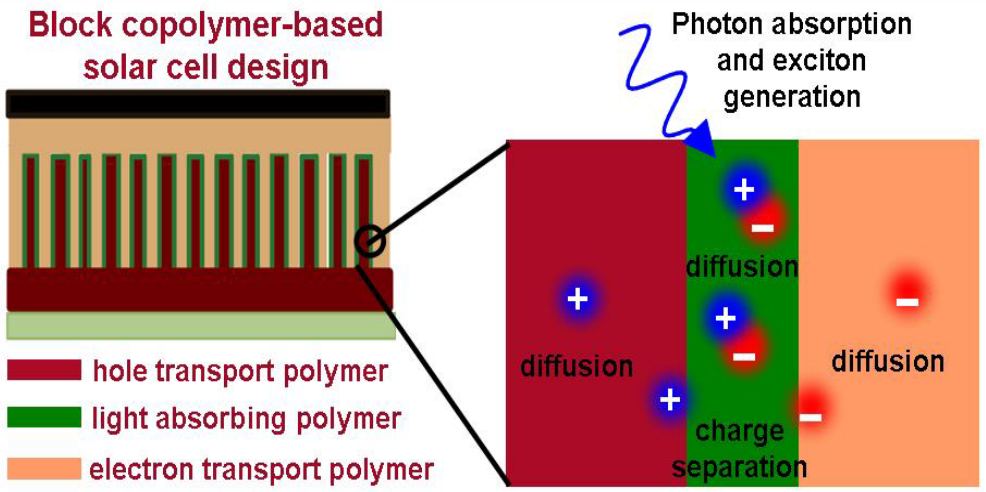
Approaches: Combination of modeling, synthetic chemistry and electrochemistry

Unique aspects: Using PEM fuel cell with organic carriers instead hydrogen gas

Potential outcome: High-density mobile and stationary energy storage systems

Polymer-Based Materials for Harvesting Solar Energy
T. P. Russell, P. Lahti (U. Massachusetts)

Summary statement: Maximize the collection and conversion efficiency of a broad frequency range of the solar spectrum using the guided self-assembly of polymer-based materials so as to optimize the design and fabrication of inexpensive devices.



RESEARCH PLAN AND DIRECTIONS

Organic-based devices, while relatively inexpensive and easy to fabricate, have low efficiencies. They are also plagued by low long-term stability problems. We face the challenge of producing affordable, efficient and robust photovoltaic devices.

Oak Ridge National Laboratory — Managed by UT-Battelle for the Department of Energy
NREL National Renewable Energy Laboratory — Innovation for Our Energy Future
KONARKA
PENNSTATE
UMASS AMHERST
U.S. DEPARTMENT OF ENERGY | Office of Science
University of Pittsburgh
UMASS LOWELL

DOE Energy Innovation Hubs

Hubs appropriated in FY 2010:

- **Fuels from Sunlight (SC lead)**
- **Energy Efficient Building Systems Design (EERE)**
- **Modeling and Simulation for Nuclear Fuel Cycles and Systems (NE)**

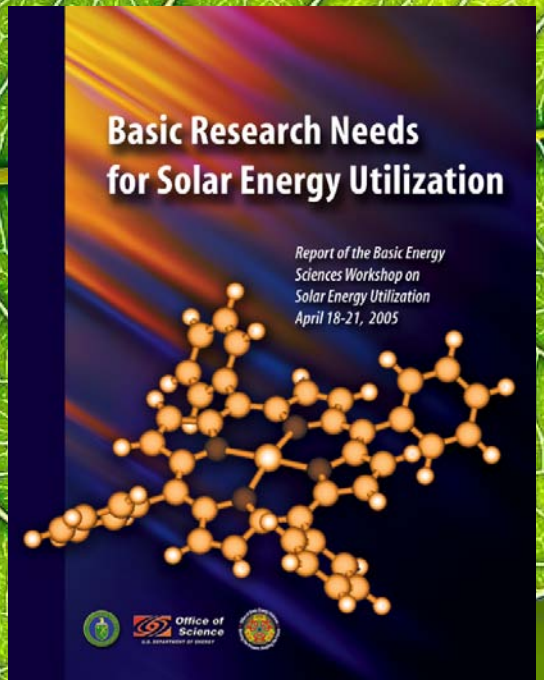
Each Hub will comprise a world-class, multi-disciplinary, and highly collaborative research and development team.

Strong scientific leadership *must* be located at the primary location of the Hub. Each must have a clear organization and management plan that "infuses" a culture of empowered central research management throughout the Hub.

The Department hopes to add additional Hubs in FY 2011.

Fuels from Sunlight: A Hub Approach?

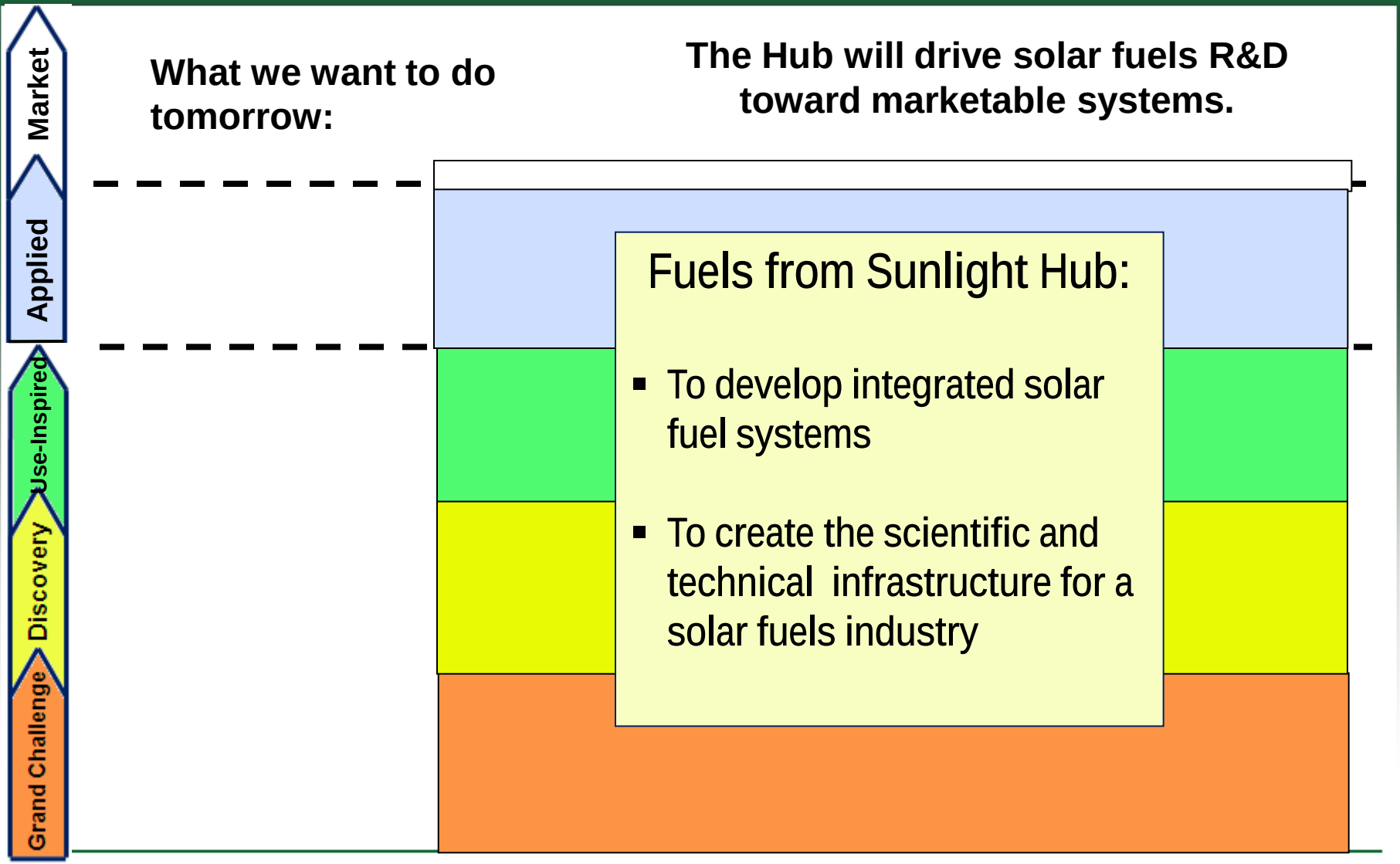
Take the "Beat-the-Leaf" Challenge



Fuels from Sunlight: Critical Issues in Research

fs	ps-ns	μs-ms
Photon absorption and harvesting	**Charge separation and transport**	**Photocatalysis**
How do we control light harvesting to utilize all of the photons?	*How do we avoid recombination of photo-generated charge carriers?*	*How do we produce fuels with the energy provided by visible light absorption?*
-Need to know how to design and control exciton transfer in molecular systems	-Need to overcome geminate recombination in organic systems	-Need hetero/homo - geneous catalytic systems for water splitting
-Need red absorbers to harvest the bulk of the solar spectrum	-Need to design transport to reduce non-geminate recombination in all systems	-Need to couple light absorption to catalytic processes for C-C bond formation

Landscape for Solar Fuels Production: From Basic Research to Market

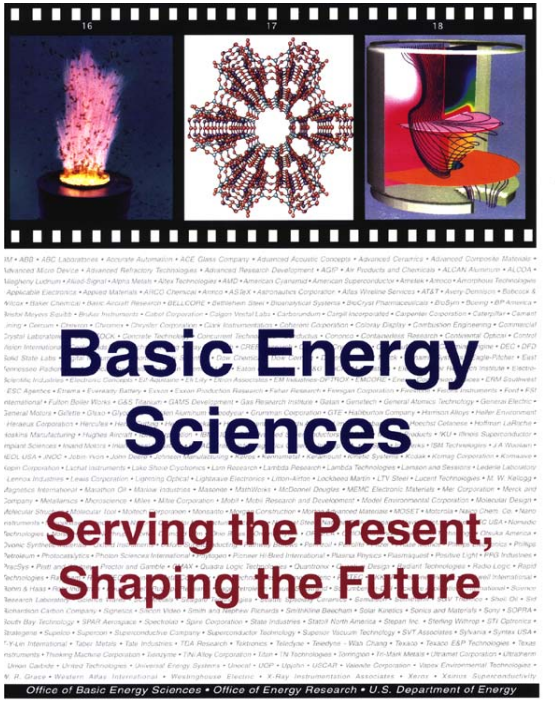


DOE Energy R&D Program Features

	Investigators and their institutions	Central location?	Diversity of Disciplines Per Award	Period of Award and Management	Award Amount	Core Motivation
Energy Innovation Hubs	Large set of investigators spanning multiple science and engineering disciplines and possibly including other non-science areas such as energy policy, economics, and market analysis. May be led by Labs or universities, nonprofit organizations or private firms. The model is the three existing Office of Science Bio-energy Research Centers.	Lead institution must provide a central location and strong scientific leadership. There must be a culture of empowered central research management.	Many	Five years with 5-year renewal possible; the "bar" is significantly higher for further renewals. Managed by Offices across DOE. A Board of Advisors consisting of senior leadership will coordinate across DOE.	~$22 million in the first year with up to $10 million for infrastructure start-up; ~$25 million per year in subsequent years.	Integrate from fundamental research through potential commercialization. The breadth and emphasis of activities will be influenced by the nature of the Hub. Some Hubs may place a greater emphasis on basic and applied research, while others may focus more on technology development. DOE determines the topical areas of the Hubs and FOAs are topic-specific.
Energy Frontier Research Centers	Self-assembled group of ~6-12 investigators. May be led by DOE laboratories or universities. About two thirds of 46 EFRCs are led by universities.	Mostly multi-institutional centers, but with a clearly defined lead institution responsible for management.	Several	Five years with 5-year renewal possible. Managed by the Basic Energy Sciences program in the DOE Office of Science.	$2-5M/year	Fundamental research with a link to new energy technologies or technology roadblocks. The investigators proposed the subject matter from among a large set of scientific grand challenges and energy-relevant topics identified in and the FOA.
ARPA-E	Single investigator, small group, or small teams.	Variable depending on project	Few	1-3 years Managed by ARPA-E, which reports to the Secretary of Energy	$0.5 - 10M/year	High risk translational research driven by the potential for significant commercial impact in the near-term. In general, DOE determines the topics of interest, except for the initial FOA, which was broad-based.

Connecting Basic and Applied Science

- **Workshop and report planned: Science for National Need – Bringing forefront scientific knowledge and state-of-the-art tools to solving grand energy challenges**
  - **To explore basic science research that is coupled more closely to industry or applied science needs.**
  - **Identify grand science challenges that will have transformational**



- **BES Overview Brochure summarizes research has had commercial and national impact**
  - Revision underway

Funding Opportunities: FAQs

- **How do I get DOE/BES support?**
  - Respond to “Open Call For Proposals” (go to grants.gov).
  - Hypothesis driven, fundamental science project - energy relevance.
  - White papers/pre-proposals are encouraged but not required.
  - All proposals peer reviewed.

- **How much support can I get?**
  - How much support do you need? (10 CFR 605)

- **How long will it take for me to find out if my project is funded?**
  - Open call is a continuous process (no fixed deadline for submission).
  - Reviews take 4 – 6 months to complete, awards are made base on strength of the merit review and available resources.
  - Proposals can be held up to one year for consideration.

Review and Selection of Research Projects

All research projects supported by the Office of Basic Energy Sciences (BES) undergo regular peer review and merit evaluation based on procedures set down in 10 CFR Part 605 for the extramural grant program

1) **Scientific and/or technical merit of the project;**- for example, the influence that the results might have on the direction, progress, and thinking in relevant scientific fields of research; the likelihood of achieving valuable results; and the scientific innovation and originality indicated in the proposed research.

2) **Appropriateness of the proposed method or approach**;- for example, the logic and feasibility of the research approaches and the soundness of the conduct of the research.

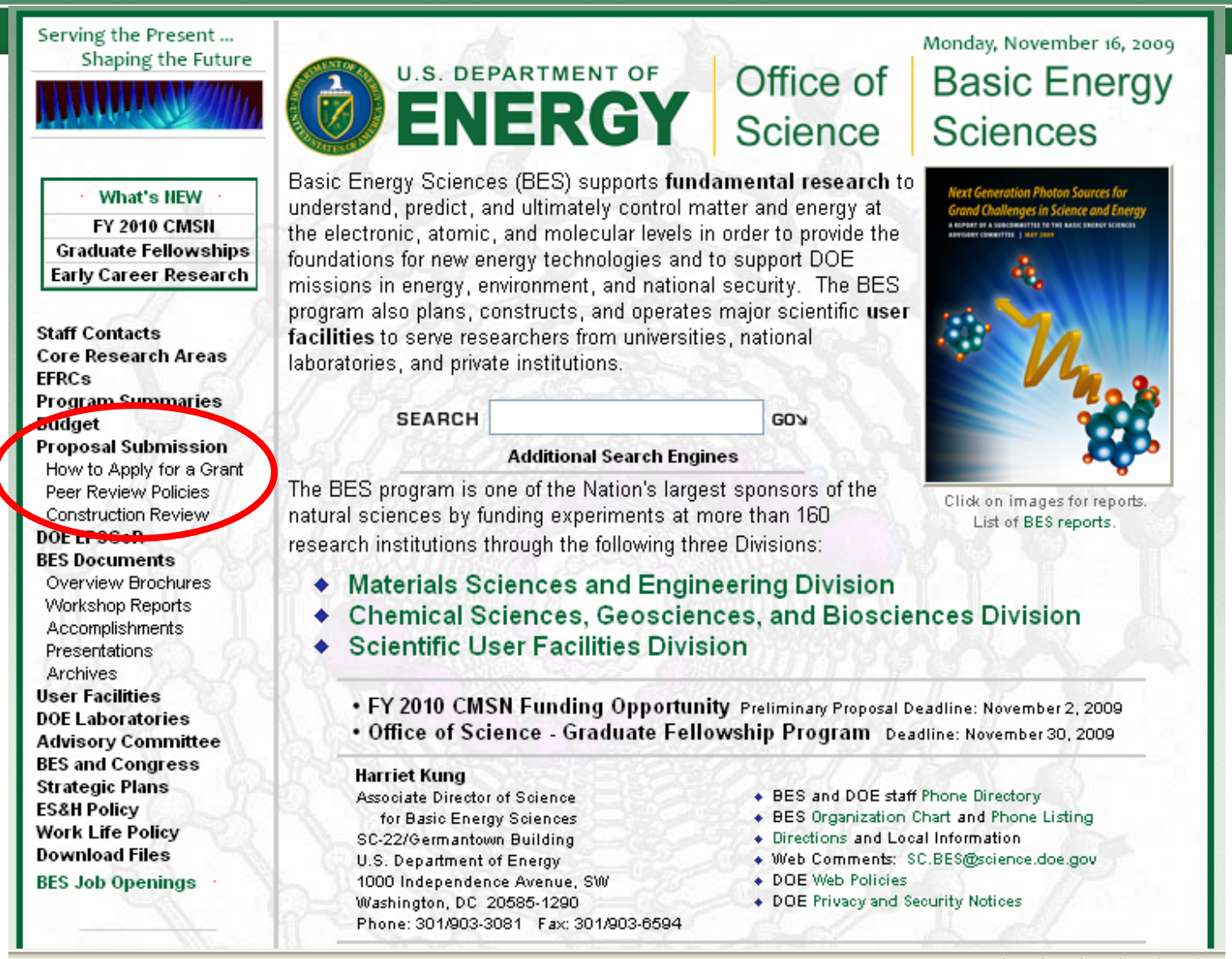
3) **Competency of the personnel and adequacy of proposed resources**; and- for example, the background, past performance, and potential of the investigator(s); and the research environment and facilities for performing the research.

4) **Reasonableness and appropriateness of the proposed budget**.

Office of Science (SC) Merit Review System

- SC Grant Application Guide
- 10 CFR Part 605

More Information? www.sc.doe.gov/bes/ *



* Or just Google "DOE + BES"

Questions?