U.S. DEPARTMENT OF ENERGY

Materials Sciences and Engineering Division Overview

University Materials Council Meeting

June 20, 2011

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

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

Under Secretary for Science
Steven E. Koonin

Office of Science
William Brinkman
Patricia Dehmer

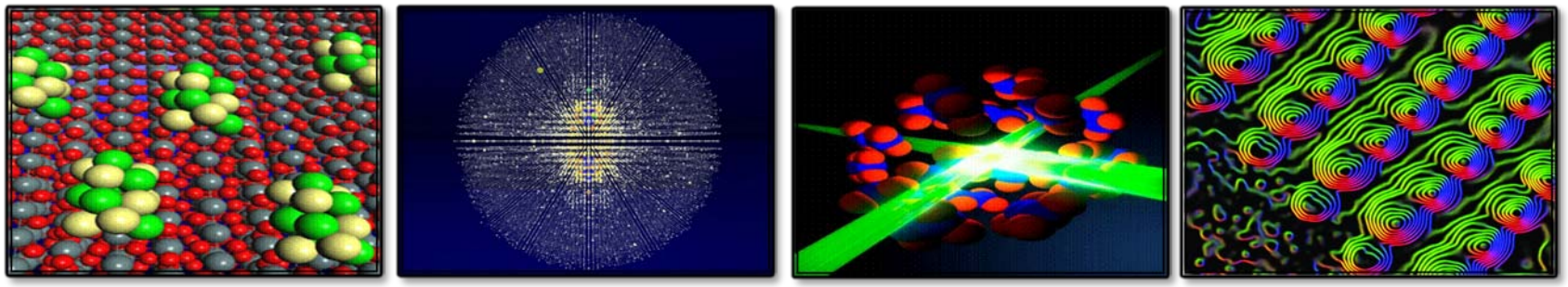
- **Basic Energy Sciences** — Harriet Kung
- **High Energy Physics** — Mike Procario (A)
- **Advanced Scientific Computing Research** — Dan Hitchcock (A)
- **Nuclear Physics** — Tim Hallman
- **Biological & Environmental Research** — Sharlene Weatherwax
- **Fusion Energy Sciences** — Ed Synakowski
-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

Under Secretary
Arun Majumdar (A)

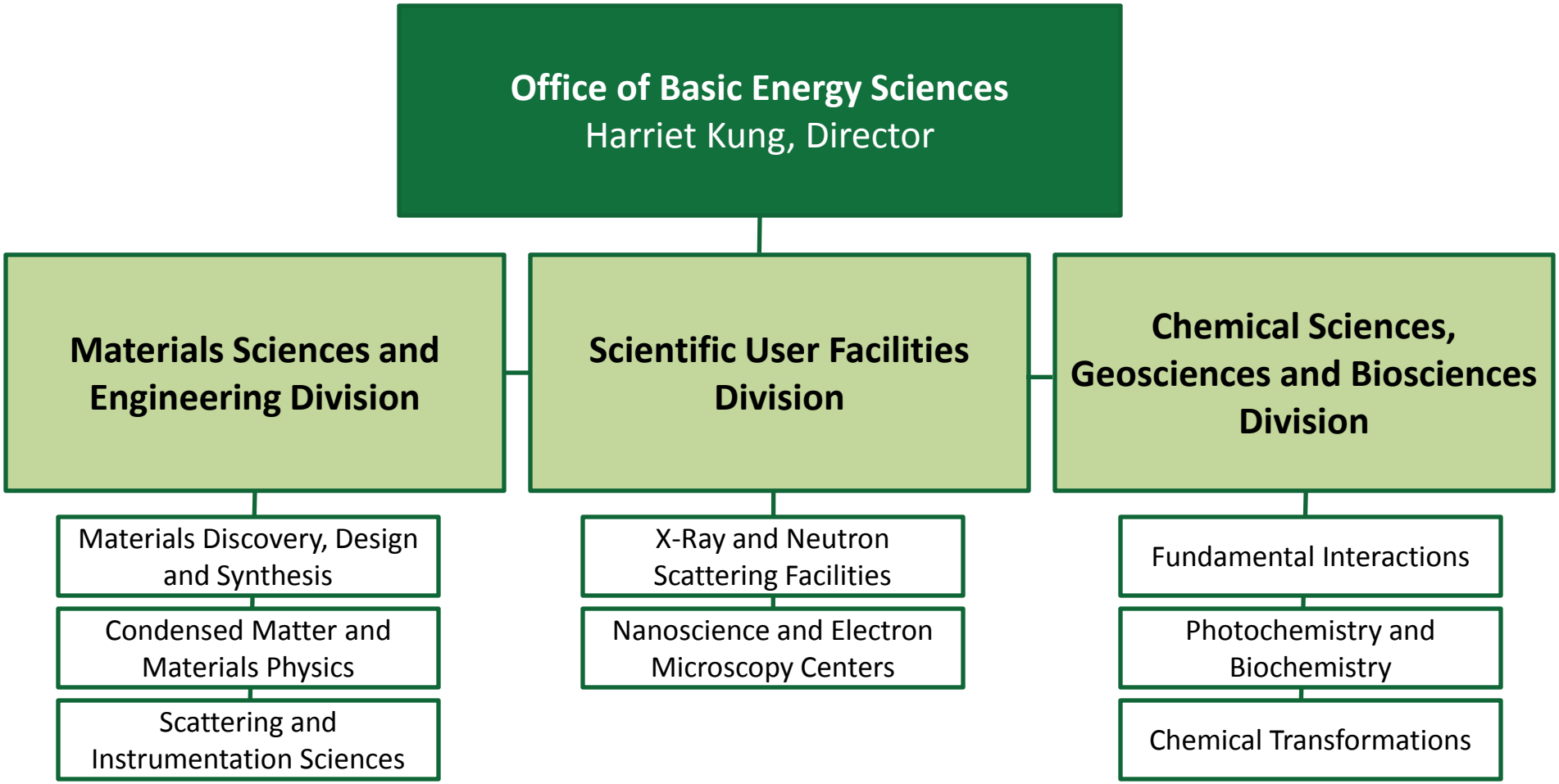
- **Energy Efficiency & Renewable Energy** — Henry Kelley (A)
- **Fossil Energy** — Victor Der (A)
- **Nuclear Energy** — Pete Lyons
- **Electricity Delivery & Energy Reliability** — Pat Hoffman

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



Office of Basic Energy Sciences

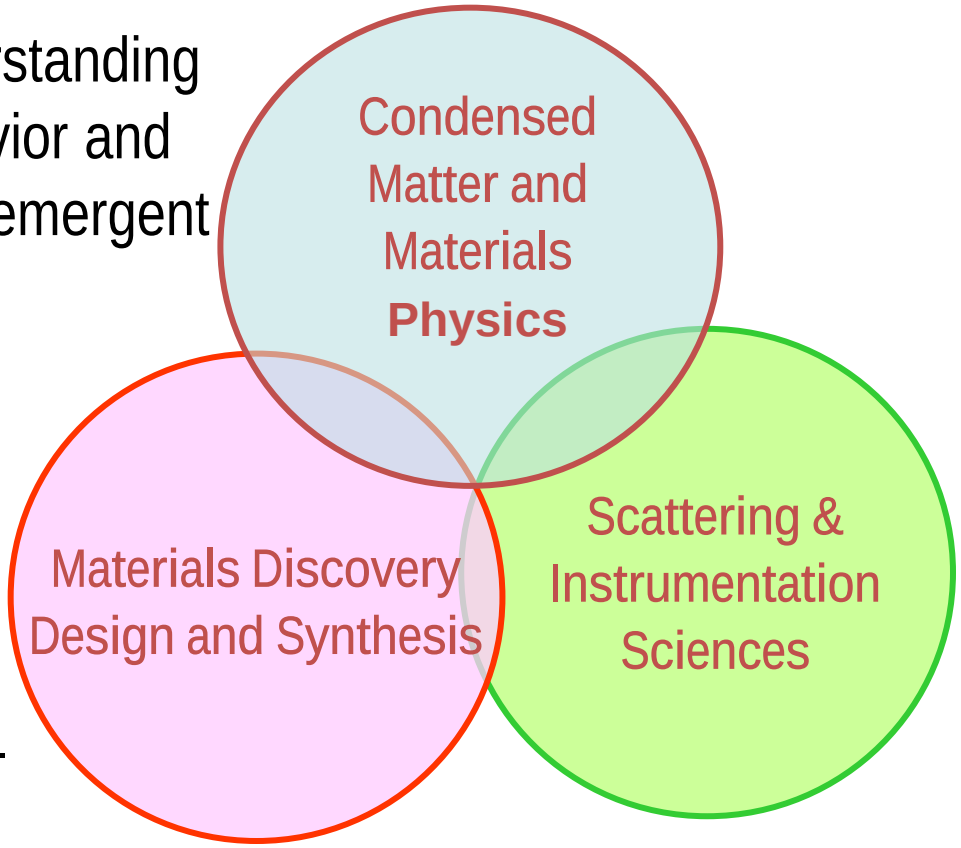


Research grouped by scientific topics
-- not by specific energy technologies

Materials Sciences and Engineering Research Focus Areas

Control and understanding of materials behavior and discovery of new emergent phenomena

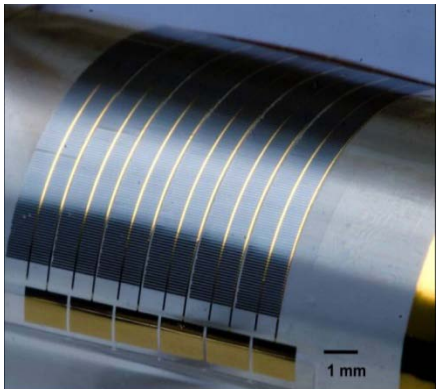
Rational design and synthesis of new materials via physical, chemical, and bio-molecular routes



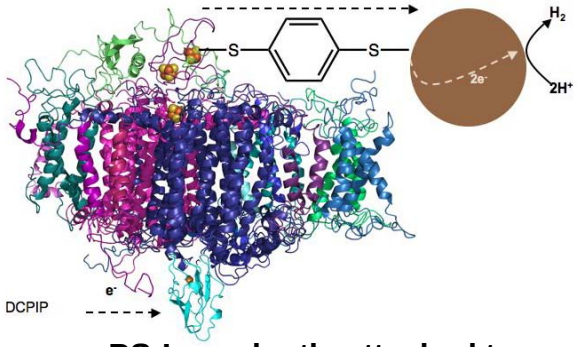
Study of photon, neutron, and electron interactions with matter for characterization of materials structures and excitation.

Division-wide themes: strongly correlated electron systems; materials synthesis; nanoscale science; theory, modeling, & simulation

Materials Discovery, Design, and Synthesis



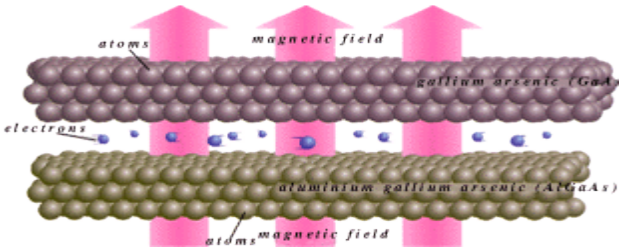
Flexible solar cells with efficiencies of ~12% and silicon thicknesses of 15 μm



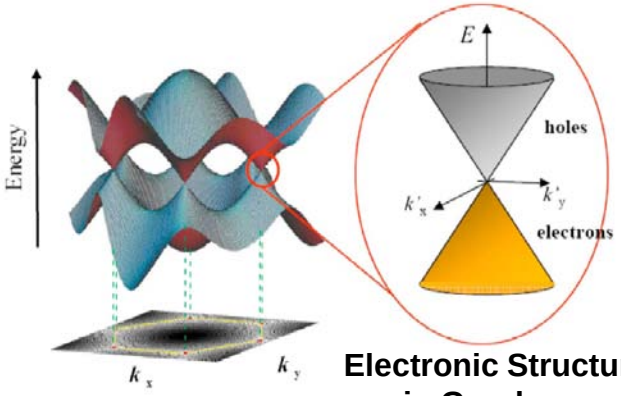
PS-I covalently attached to nanoparticle catalysts via a molecular wire yields 75% of plant electron transfer rates resulting in photo-generated hydrogen at ~1700 X current benchmarks

- **Synthesis and Processing Science**
  - Learn to control synthesis and processing by developing scientific foundations, *in situ* studies, and for a wide range of materials
- **Biomolecular Materials**
  - Discovery, design and synthesis of biomimetic and bioinspired functional materials and energy conversion processes based on principles and concepts of biology
- **Materials Chemistry**
  - Nanoscale chemical synthesis and assembly; solid state chemistry; novel polymeric materials and complex fluids; surface and interfacial chemistry

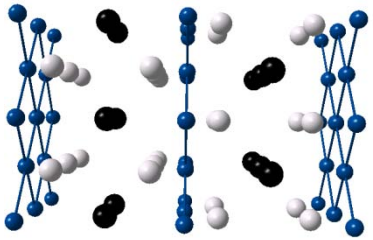
Condensed Matter and Materials Physics



Two-Dimensional Electrons in Gallium Arsenide Semiconductors



Electronic Structure in Graphene

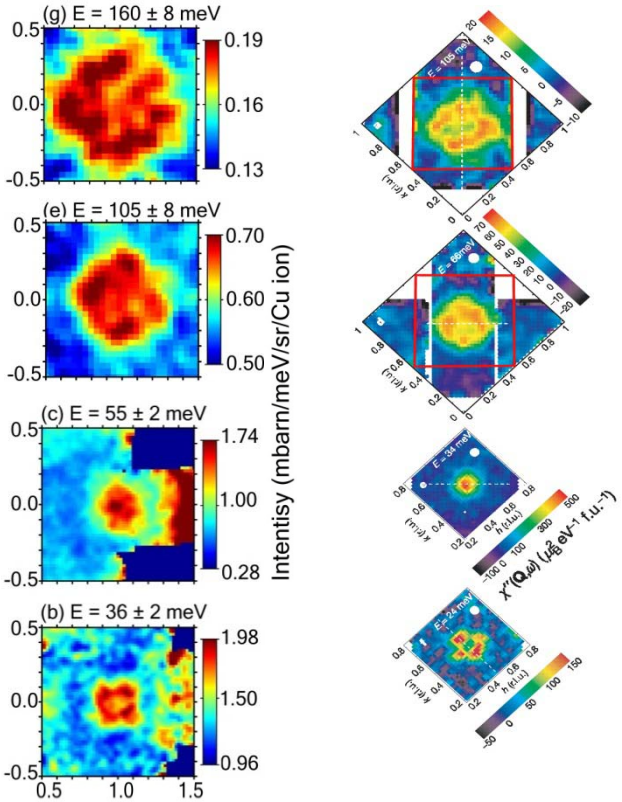


Tetragonal structure with square nets of $Fe^{2+\delta}$ in $BaFe_{1.84}Co_{0.16}As_2$

- **Experimental Condensed Matter Physics**
  - Fundamental understanding of condensed matter phenomena including correlated electron behavior on properties of materials
- **Theoretical Condensed Matter Physics**
  - Theory, modeling, and simulation of condensed phase matter emphasizing electronic correlations, nanoscale phenomena
- **Mechanical Behavior and Radiation Effects**
  - Understand defects and their impact on materials properties, including their extreme to environments
- **Physical Behavior of Materials**
  - Understand relationships of material phenomena to external environment emphasizing thermal and optical properties

Scattering and Instrumentation Sciences

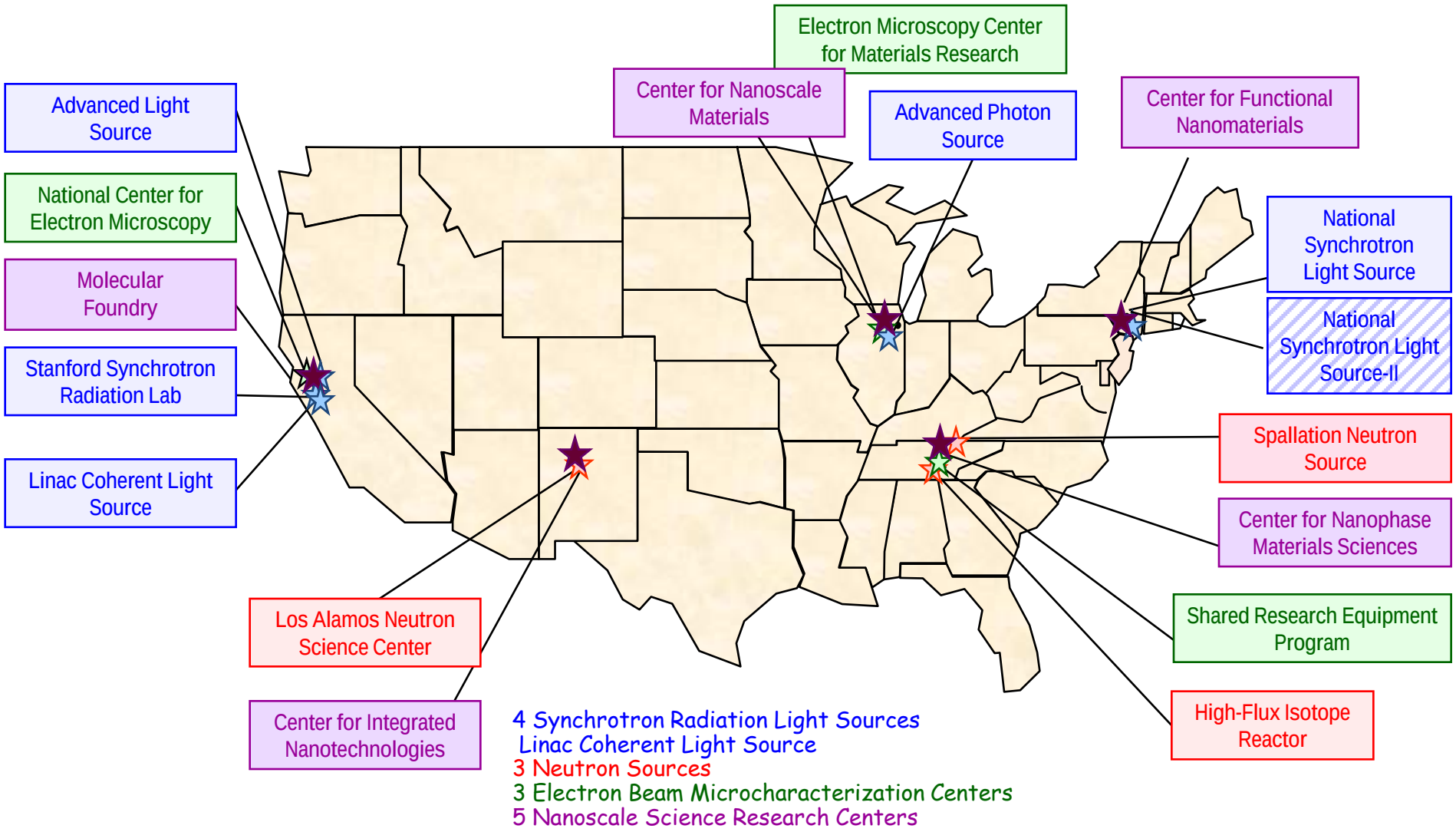
Magnetic Fluctuations in Superconductors



Neutron scattering studies demonstrate universal magnetic excitation spectrum

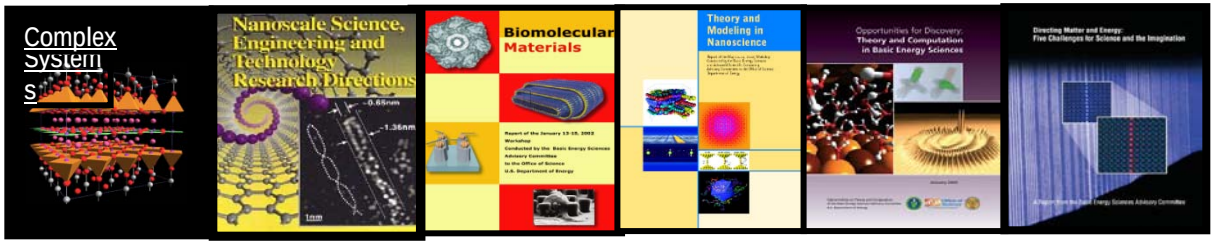
- **X-Ray and Neutron Scattering**
- **Electron and Scanning Probe Microscopies**
  - Utilize scanning probes to elucidate mechanisms that control phenomena
- Complements research performed at major BES user facilities
- Unify the complementary information obtained through multiple techniques
- Develop a structural and dynamical understanding of nanostructured materials
- Understand dynamics and materials functionality using ultrafast diffraction, spectroscopy and imaging techniques

BES Scientific User Facilities: Resources for Research



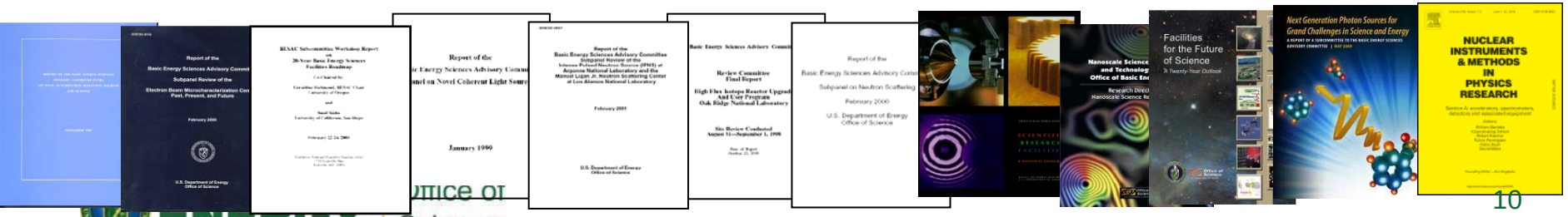
BES Strategic Planning Activities

- *Science for Discovery*



- *Science for National Needs*

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



Recurring Themes - BES Strategic Planning

>>1,500 participants from academia, industry, and federal labs

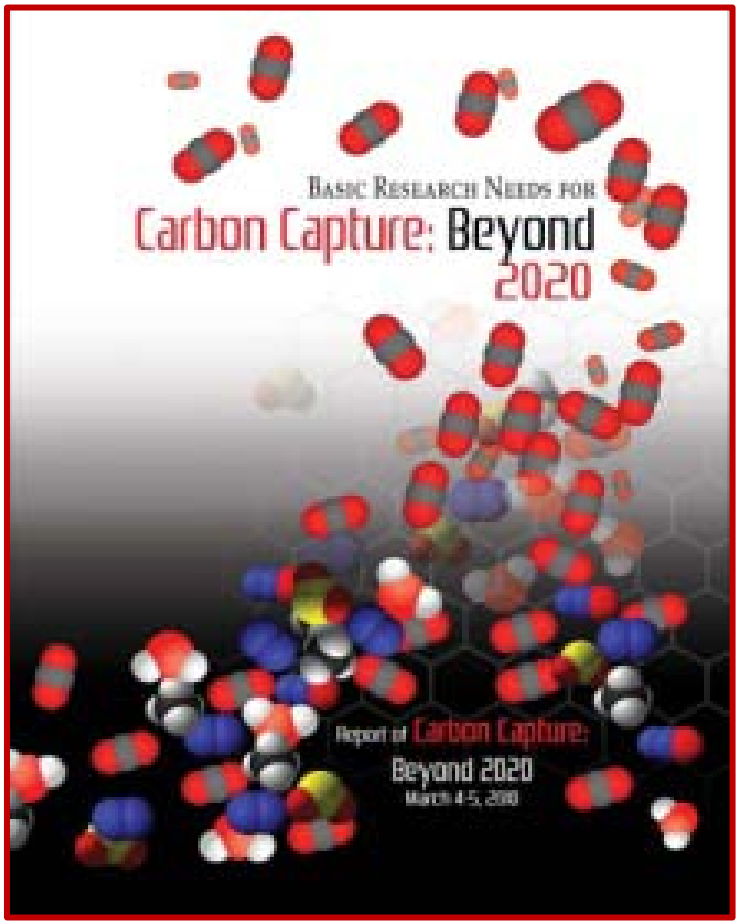
Disruptive, Transformational Advances Require "Control"

Control of materials properties and functionalities through electronic and atomic design

- New materials discovery, design, development, and fabrication, especially materials that perform well under extreme conditions
- "Control" of photon, electron, spin, phonon, and ion transport in materials
- Science at the nanoscale, especially low-dimensional systems
- Designed catalysts
- Designed interfaces and membranes
- Structure-function relationships
- Bio-materials and bio-interfaces, especially at the nanoscale
- New tools for spatial characterization, temporal characterization, and for theory/modeling/computation

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

Carbon Capture Beyond 2020



Organized by BES and Fossil Energy

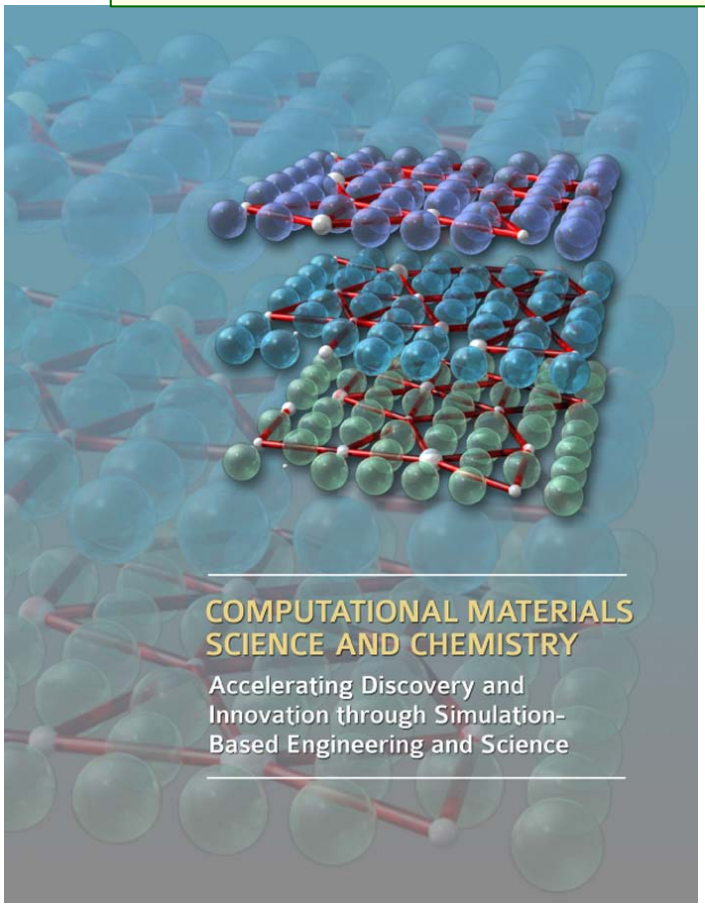
- **Thermodynamically efficient and scalable carbon capture stands as one of the greatest challenges for energy**
- **Priority Research Areas**
  - Understand and control the dynamic atomic-level and molecular-level interactions of the targeted species with the separation media
  - Discover and design new materials that incorporate designed structures and functionalities tuned for optimum separation properties
  - Tailor capture/release processes with alternative driving forces, taking advantage of a new generation of materials.
  - New analytical tools to characterize materials structure and molecular processes across broad spatial and temporal scales
  - Computational tools for theory, modeling, and simulation of separation processes

http://science.energy.gov/bes/news-and-resources/reports/abstracts/

Computational Materials Science and Chemistry

Creating an Innovation Ecosystem

"We are at the threshold of a new era where predictive modeling will transform our ability to design new materials and chemical processes, thereby enabling rational discovery strategies for systems that were not tractable a few years ago."



- Integration of synthesis, processing, characterization, theory, and simulation and modeling.
- Achieving/strengthening predictive capability in foundational challenge areas.
- Developing validated computational approaches that span vast differences in time and length scales.
- Experimental validation and quantification of uncertainty in simulation and modeling.
- Robust and sustainable computational infrastructure, including software and applications.
- Efficient transfer and incorporation of simulation-based engineering and science in industry.

http://science.energy.gov/bes/news-and-resources/reports/abstracts/

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 (1 in BES)**

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

Energy Frontier Research Centers

Tackling Our Energy Challenges in a New Era of Science

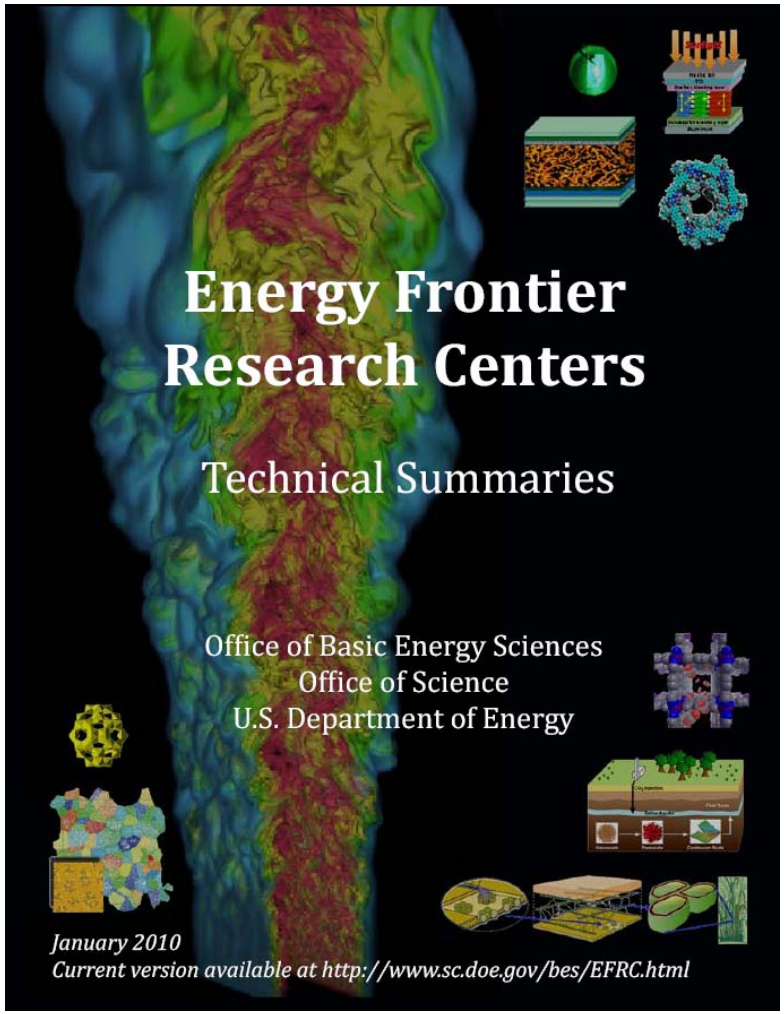
- To engage the talents of the nation's researchers for the broad energy sciences
- To accelerate the scientific breakthroughs needed to create advanced energy technologies for the 21st century
- To pursue the fundamental understanding necessary to meet the global need for abundant, clean, and economical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

46 centers awarded ($777M over 5 years) in FY2009, 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

EFRCs Technical Summaries



Two-page technical summaries provided by EFRCs PLUS

- EFRC contact information and
- Indexed by
  - investigator, institution,
  - basic research needs,
  - grand challenges,
  - topical keywords,
  - experimental and theoretical methods

Available and downloadable on-line – Revised for FY 2011

Science for Our Nation's Energy Future:

- Explored the challenges and opportunities in applying America's extraordinary scientific and technical resources to critical energy needs
- Highlighted early successes of the Office of Science Energy Frontier Research Centers
- Promoted collaboration across the national energy enterprise

Over 1,000 Participants including:

- Leaders from science, industry and government from the US and abroad
- Students, young researchers, and senior investigators
- Members of the media and the general public

Highlights:

- Invited speakers included: **Steven Chu** – US Secretary of Energy; **John Hennessy** – President of Stanford University; **Mark Little** – Senior VP and Director of GE Global Research; and **Eric Isaacs** – Director of Argonne National Laboratory
- Screening of the winners of *Life at the Frontiers of Energy Research* video competition
- Keynote speakers, parallel technical sessions, and poster presentations on the scientific issues and promising opportunities of a wide range of energy topics

DOE Energy Innovation Hubs

Hubs funded in FY 2010:

- **Fuels from Sunlight (SC lead) – CalTech- LBNL**
- **Energy Efficient Building Systems Design (EERE) – Penn State**
- **Modeling and Simulation for Nuclear Fuel Cycles and Systems (NE) - ORNL**

Each Hub has a world-class, multi-disciplinary, and highly collaborative research and development team

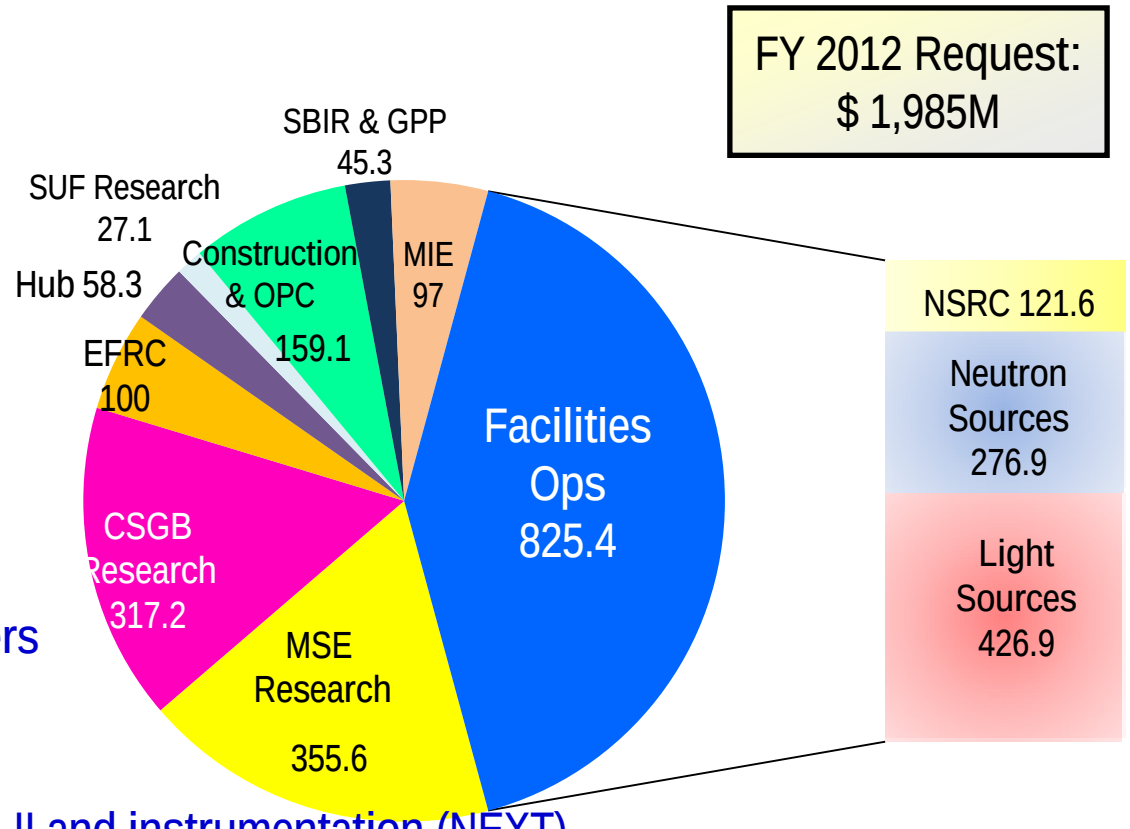
Strong scientific leadership *is* located at the primary location of the Hub.

- **Clear organization and management plan**
- **"infuses" a culture of empowered central research management**

The Department has proposed three additional Hubs, including for Batteries and Energy Storage.

FY 2012 BES Budget Request

- Research programs
  - Energy Innovation Hubs
  - Energy Frontier Research Centers
  - Core Research: increases in basic research for energy; materials by design; nanoelectronics; methane hydrates
- Scientific user facilities operations
  - Synchrotron light sources
  - Neutron scattering facilities
  - Nanoscale Science Research Centers
  - Instrumentation for clean energy
- Construction and instrumentation
  - National Synchrotron Light Source-II and instrumentation (NEXT)
  - Spallation Neutron Source instruments & power upgrade
  - Advanced Photon Source upgrade
  - Linac Coherent Light Source-II
  - TEAM-II



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

- Improved energy storage is critical for the widespread use of intermittent renewable energy, electric vehicles, and efficient and reliable smart electric grid technologies.
- The proposed Hub will develop electrochemical energy storage systems that safely approach theoretical energy and power densities with very high cycle life.
- These are systemic challenges requiring new materials, systems, and 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?
- The Hub will link fundamental science, technology, and end-users, and it will collaborate with relevant Energy Frontier Research Centers, ARPA-E, OE, and EERE

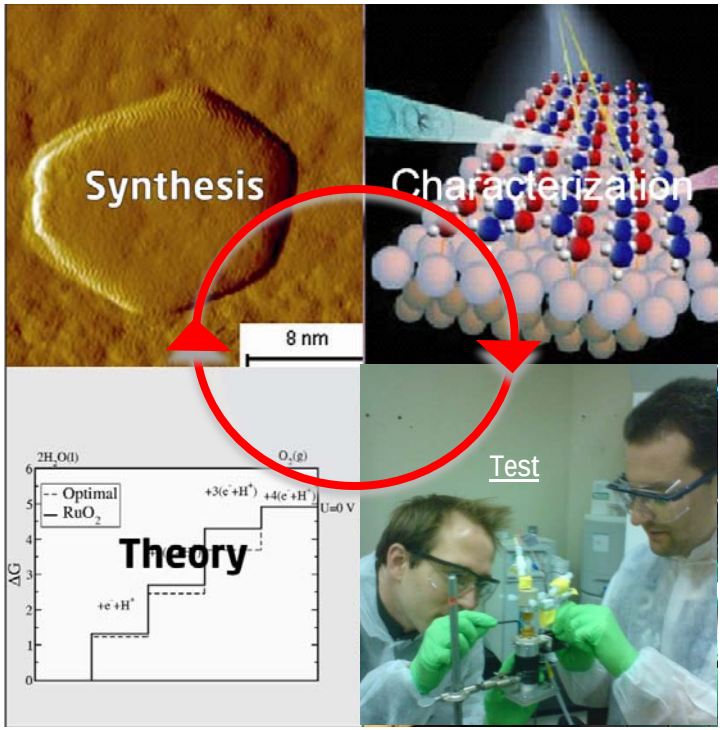
Materials by Design

- Research to establish materials design rules to launch an era of predictive modeling, changing the paradigm of materials discovery from serendipity to rational design.
- Discovery of new materials has been the engine driving science frontiers and fueling technology innovations. The U.S. has the world's most powerful suite of tools for materials synthesis, characterization, and computation.
- $40M request to support the following research focus:

Synthesis: Rational molecular-scale design guided by simulation.

Characterization and Testing: Verify & validate computational designs and software, including in situ measurements using x-ray, neutron, microscopy, and nanoscience facilities.

Theory/Simulation: New methods and algorithms for complex, multi-scale systems. Development of software and toolkits through a networked, broad community. Emphasis areas include: catalysis, light-weight materials, and materials for energy applications including radiation-resistant materials, carbon capture, batteries, liquid fuels, and photocatalysis.



FY12 Budget Request: Science for Energy

Non-carbon Sources	(Dollars in thousands)
Solar Electricity from Photovoltaics	+ 8,000
Advanced Nuclear Energy Systems	+ 8,000
Materials under Extreme Environments	+15,000
Carbon Capture and Sequestration	
Carbon Capture	+ 8,000
Carbon Sequestration	+ 8,000
Transportation and Fuel Switching	
Energy Systems Simulation - Combustion	+ 15,000
Batteries and Energy Storage Hub	+ 34,020
Transmission and Energy Storage	
Electric Power Grid–Enabling Materials Sciences	+ 4,000
Power Electronics	+ 3,500
Batteries and Energy Storage Hub	(same as above)
Efficiency	
Advanced Solid-state Lighting	+ 8,000
Energy Efficiency – Enabling Materials Sciences	+ 4,000

Office of Science Early Career Research Program

To support individual research programs of outstanding scientists early in their careers and to stimulate research careers in the disciplines supported by the Office of Science

Eligibility: Within 10 years of receiving a Ph.D., either untenured academic assistant professors on the tenure track or full-time DOE national lab employees

Award Size: University grants $150,000 per year for 5 years to cover summer salary and expenses

FY 2010 Results:

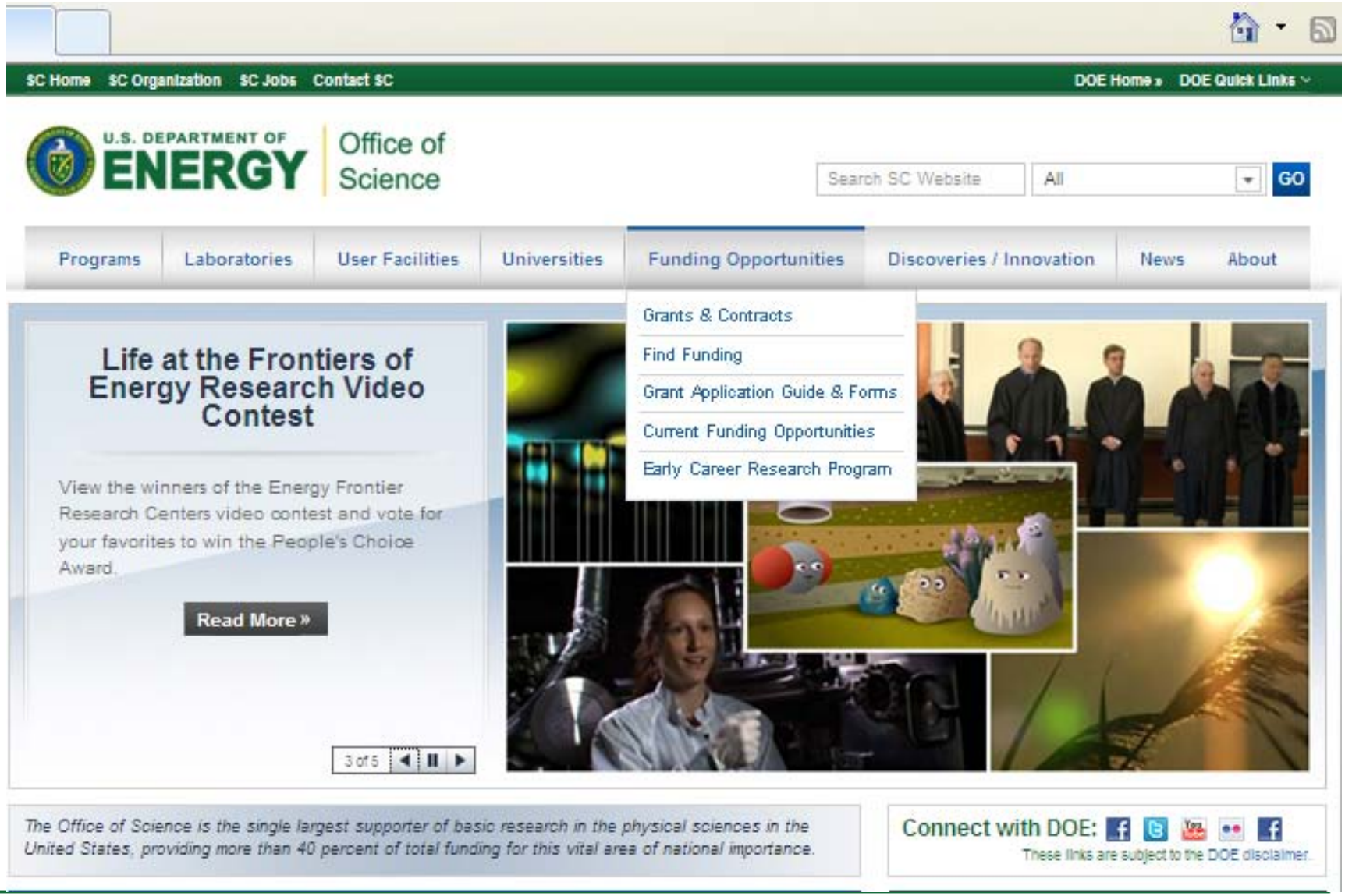
- 69 awards funded via the American Recovery and Reinvestment Act*
- 47 university grants and 22 DOE national laboratory awards

FY 2011 Application Process:

- Funding Opportunity Announcement issued in July 2010 - Pre-applications were required, full proposals have been received
- 69 Awards to date in FY 2011

FY 2012 Application Process: Should be announced soon

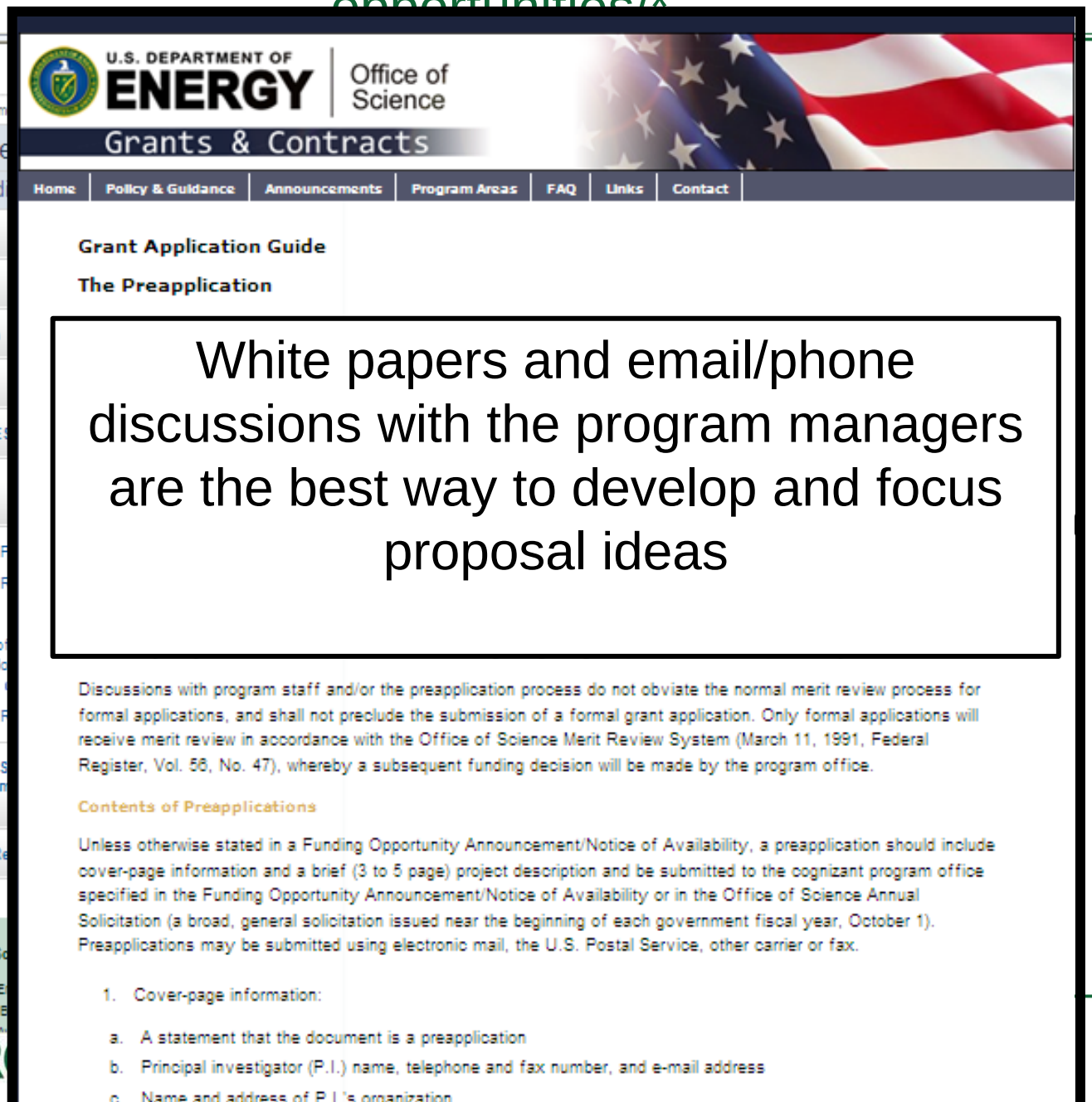
More information – Office of Science Homepage: http://science.energy.gov/



More Information? http://science.energy.gov/bes/

* Or just Google "DOE + BES"

More Information? http://science.energy.gov/bes/funding-opportunities/*



time….

Administrative Staff
Marsophia Agnant, Cheryl Howard, Jorge Mariani
Teresa Crockett , ????

Materials Sciences and Engineering Division

Linda Horton, Division Director

Materials Discovery, Design, and Synthesis Team

Team Lead - Arvind Kini

Materials Chemistry

?

Biomolecular Materials

Mike Markowitz

Synthesis & Processing Sciences

Bonnie Gersten

Integrated Energy Research

John Vetrano

Condensed Matter and Materials Physics Team

Team Lead - Jim Horwitz

Experimental Condensed Matter Physics

Andrew Schwartz

Theoretical Condensed Matter Physics

Jim Davenport

Physical Behavior of Materials

Refik Kortan

Mechanical Behavior & Radiation Effects

John Vetrano

Scattering and Instrumentation Sciences Team

Team Lead - Helen Kerch

X-ray Scattering

Lane Wilson

Neutron Scattering

Thiyaga P. Thiyagarajan

Electron and Scanning Probe Microscopies

Jane Zhu

Experimental Program to Stimulate Competitive Research

Tim Fitzsimmons

Questions?

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