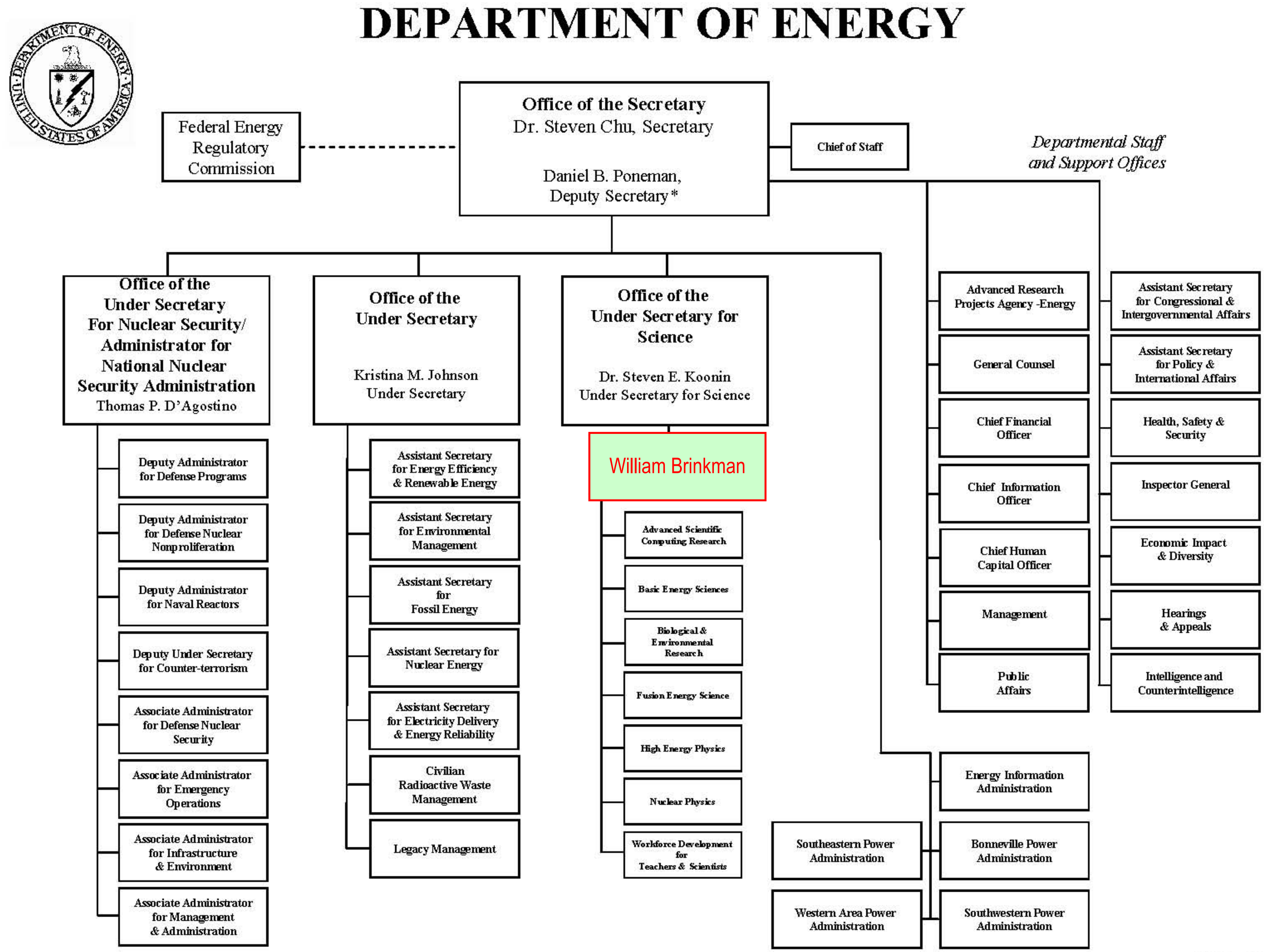
Energy Research Needs and Opportunities in Materials Sciences and Engineering

Semiconductor Research Corporation Board Meeting
July 1, 2009

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

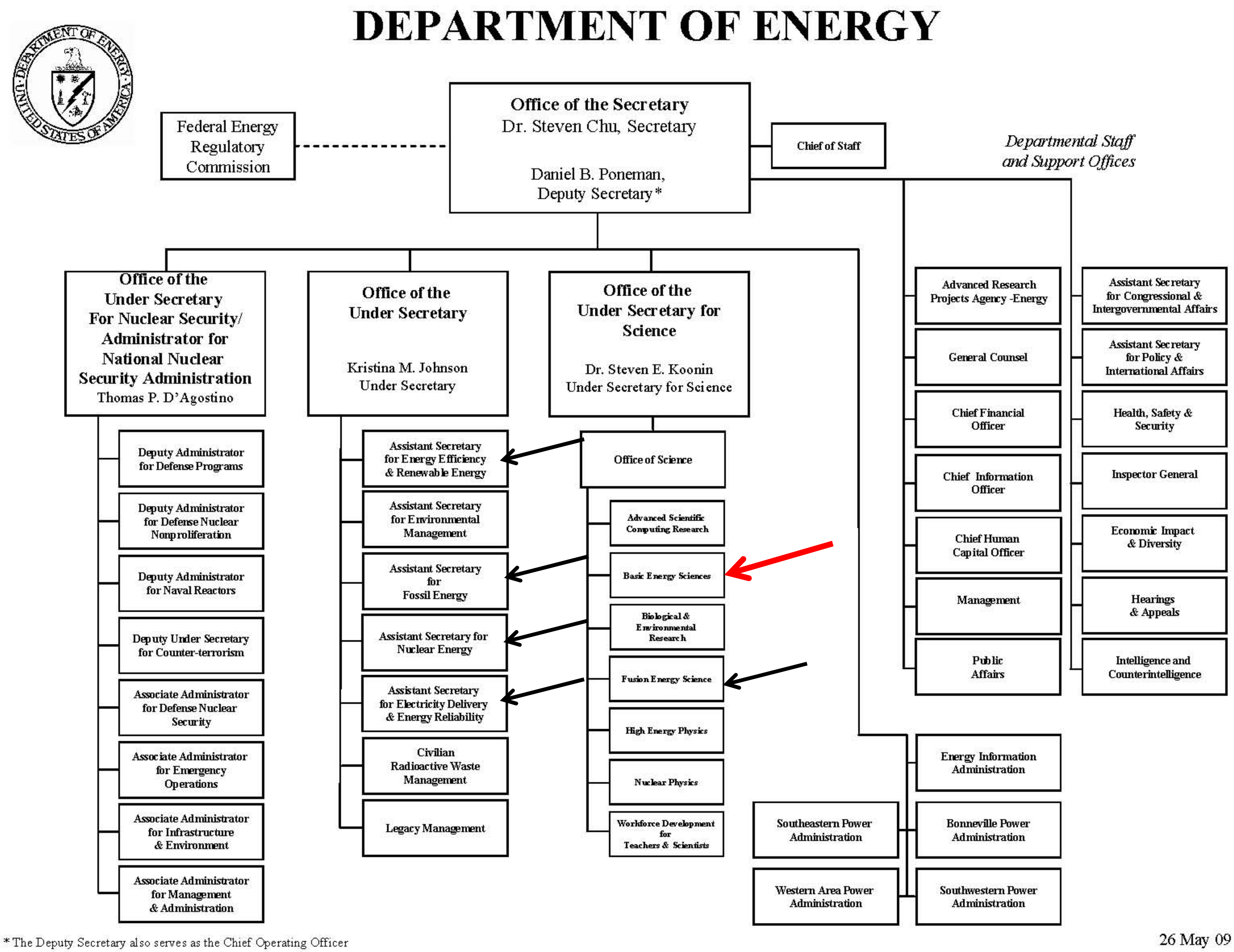
DOE – From Fundamental to Technology Specific R&D



* The Deputy Secretary also serves as the Chief Operating Officer

26 May 09

Where is Materials Sciences and Engineering R&D Supported?



Office of Basic Energy Sciences

Harriet Kung, Director
Wanda Smith, Administrative Specialist

BES Budget and Planning
- Bob Astheimer, Technical Advisor
- Margie Davis, Financial Management
- Vacant, Program Support Specialist

BES Operations
- Rich Burrow, DOE Technical Office Coordination
- Don Freeburn, DOE and Stakeholder Interactions
- Ken Rivera, Laboratory Infrastructure / ES&H
- Katie Perine, Program Analyst / BESAC
- Vacant, Technology Office Coordination

Materials Sciences and Engineering Division
Linda Horton, Director
- ◆ Ehsan Khan, Program Manager
- Christie Ashton, Program Analyst
- ☆ Charnice Waters, Secretary

Materials Discovery, Design, and Synthesis
Arvind Kini; Kerry Gorey, P.A.
- Materials Chemistry: Dick Kelley; ■ Jim McBreen, BNL; Vacant
- Biomolecular Materials: Mike Markowitz
- Synthesis and Processing: Bonnie Gersten; ● Jeff Tsao, SNL; ● Mike Coltrin, SNL
- 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.: Michael Lee; △ 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
- Nanoscience Centers & E-beam Centers: Tof Carim; Vacant
- Accelerator and Detector R&D: Vacant
- Facility Coordination, Metrics, Assessment: Van Nguyen

Construction
- Linac Coherent Light Source: Tom Brown
- NSLS II: Tom Brown
- Spallation Neutron Source Upgrades: Tom Brown
- TEAM: Vacant
- Instrument MIEs (SING, LUSI, etc.): Vacant
- Advanced Light Source User Support Building: Tom Brown

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

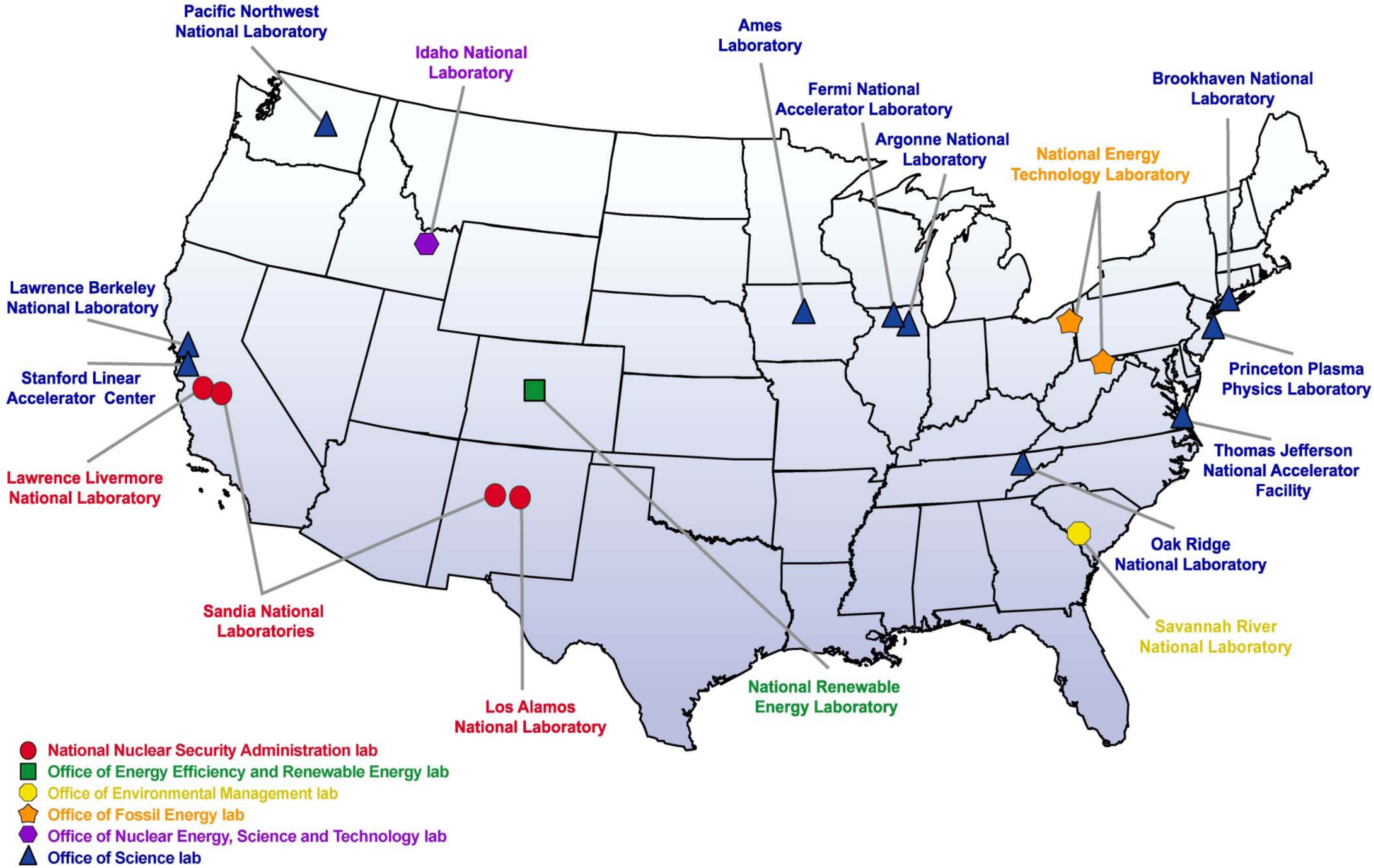
Photo- and Bio-Chemistry
Rich Greene; Sharron Watson, P.A.
- Solar Photochemistry: Mark Spitler
- Photosynthetic Systems: Gail McLean
- Physical Biosciences: Bob Stack

Chemical Transformations
John Miller; Teresa Crockett, P.A.
- Catalysis Science: Raul Miranda; Paul Maupin
- Heavy Element Chemistry: Lester Morss; ● Norm Edelstein, LBNL
- Separations and Analysis: Bill Millman; ◆ Larry Rahn, SNL
- Geosciences: Nick Woodward; ● Pat Dobson, LBNL
- 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

May 2009

DEPARTMENT OF ENERGY NATIONAL LABORATORIES



U.S. DEPARTMENT OF ENERGY

The Obama Administration's Energy & Environment Plan

- **Within 10 years save more oil than the United States currently imports from the Middle East and Venezuela combined.**
- **Put 1 million plug-in hybrid cars – cars that can get up to 150 miles per gallon – on the road by 2015.**
- **Generate 10 percent of our electricity from renewable sources by 2012, and 25 percent by 2025.**
- **Implement an economy-wide, cap-and-trade program to reduce greenhouse gas emissions 80% by 2050.**

http://www.whitehouse.gov/agenda/energy_and_environment/

Key R&D Strategies

Zero-net-emissions Electricity Generation

Fuel Switching

CCS

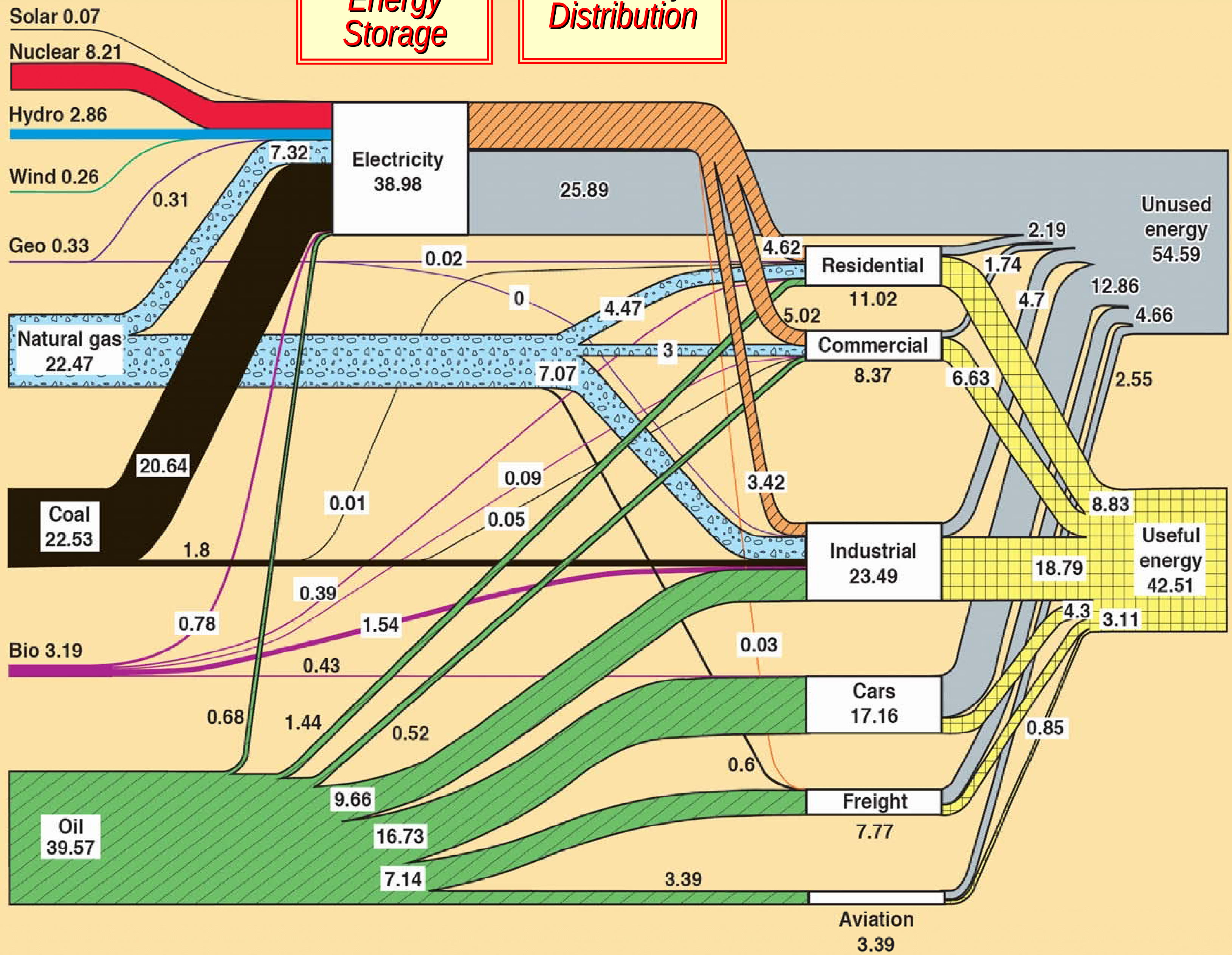
Fuel Switching

Electric Energy Storage

Electricity Distribution

End-use Efficiency

Conservation



Climate/Environment Impacts

Source: LLNL 2008; data are based on DOE/EIA-0384(2006). Credit should be given to LLNL and DOE.

Strategies: Ten "Basic Research Needs …" Workshops

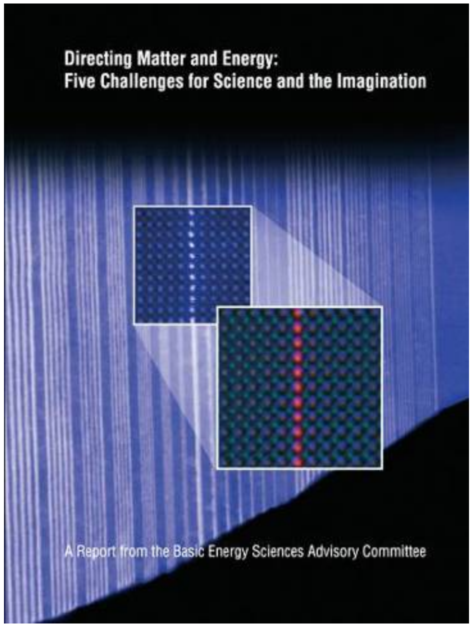
Basic Research Needs to Assure a Secure Energy Future – led by the BES Advisory Committee – followed by:

- 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

10 workshops; 5 years; more than 1,500 participants from academia, industry, and DOE labs

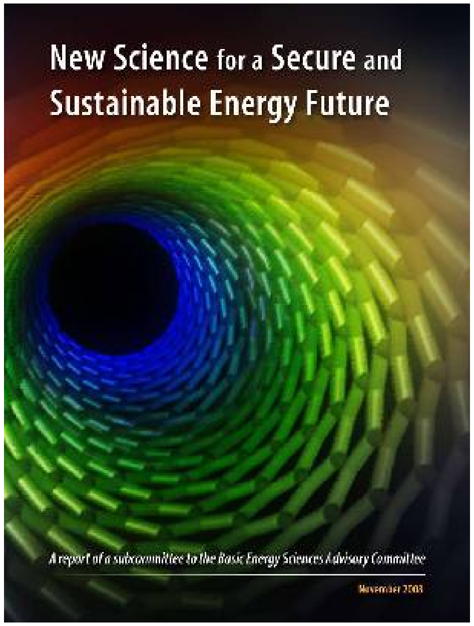
www.science.doe.gov/bes/reports/list.html

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 from the latest BES Advisory Committee Report:

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

Recommendations:

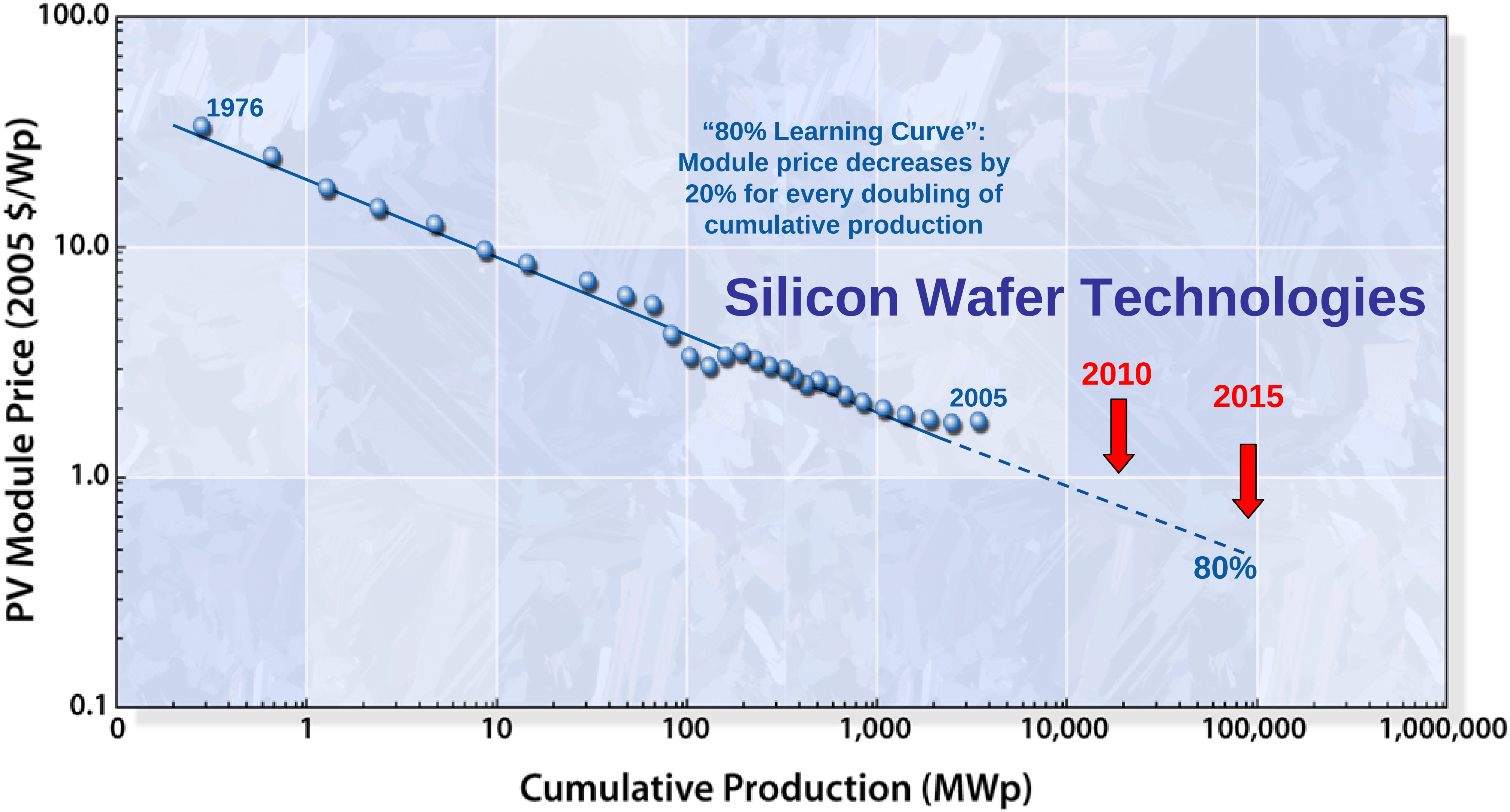
- Work at the intersection of control science and complex functional materials.
- Increase the rate of discoveries.
- Establish “dream teams” of talent, equipped with forefront tools, and focused on the most pressing challenges to increase the rate of discovery.
- Recruit the best talent through workforce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

Energy Sustainability and Materials

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 materials

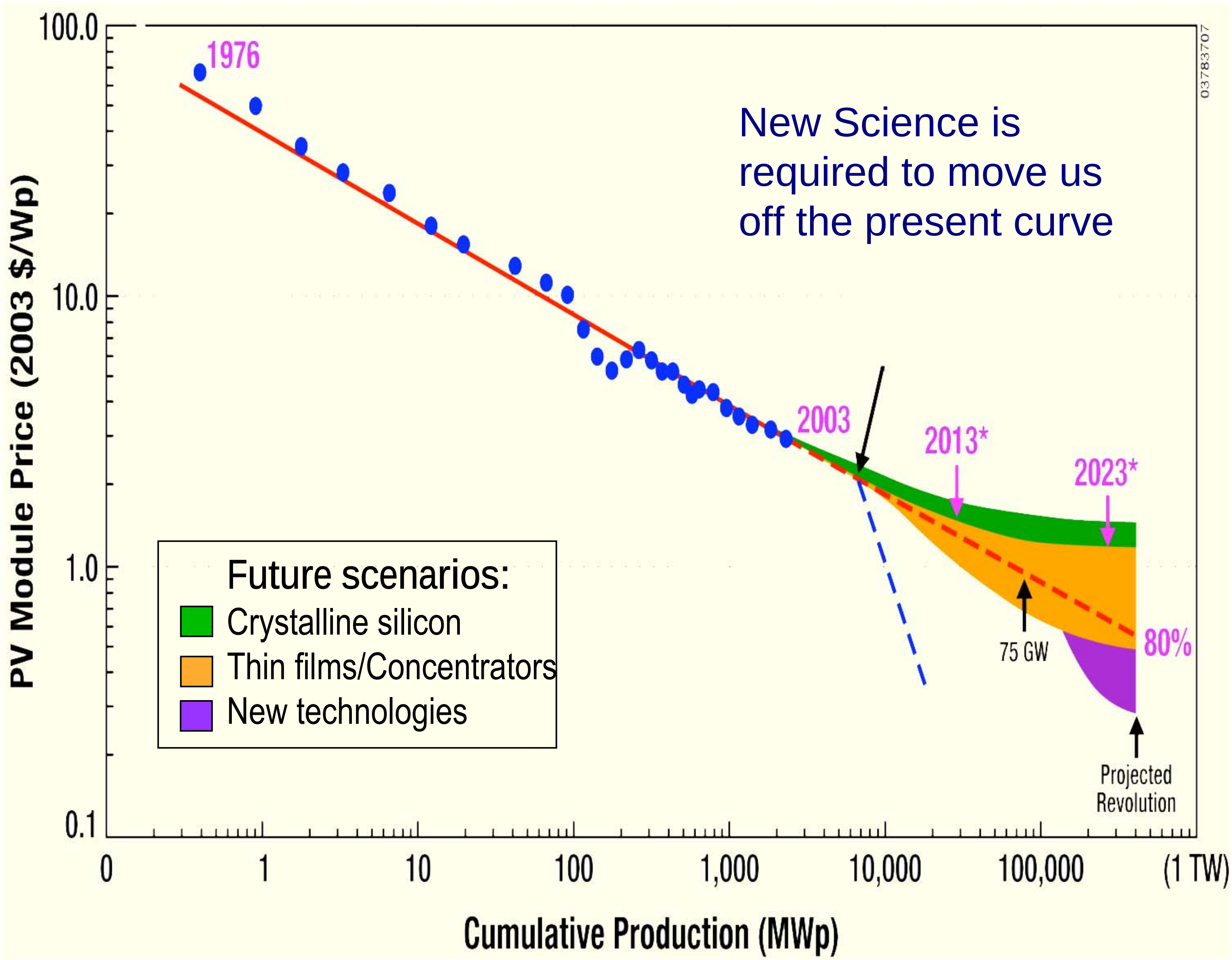
Solar Energy Utilization:
PV Production Learning Curve



Note: By 2020, current trajectory will supply 16 GW (peak) (~3.5 GW avg) in U.S. whereas at least 425 GW will be needed just for electricity, and ~2000 GW for fuel.

U.S. DEPARTMENT OF ENERGY

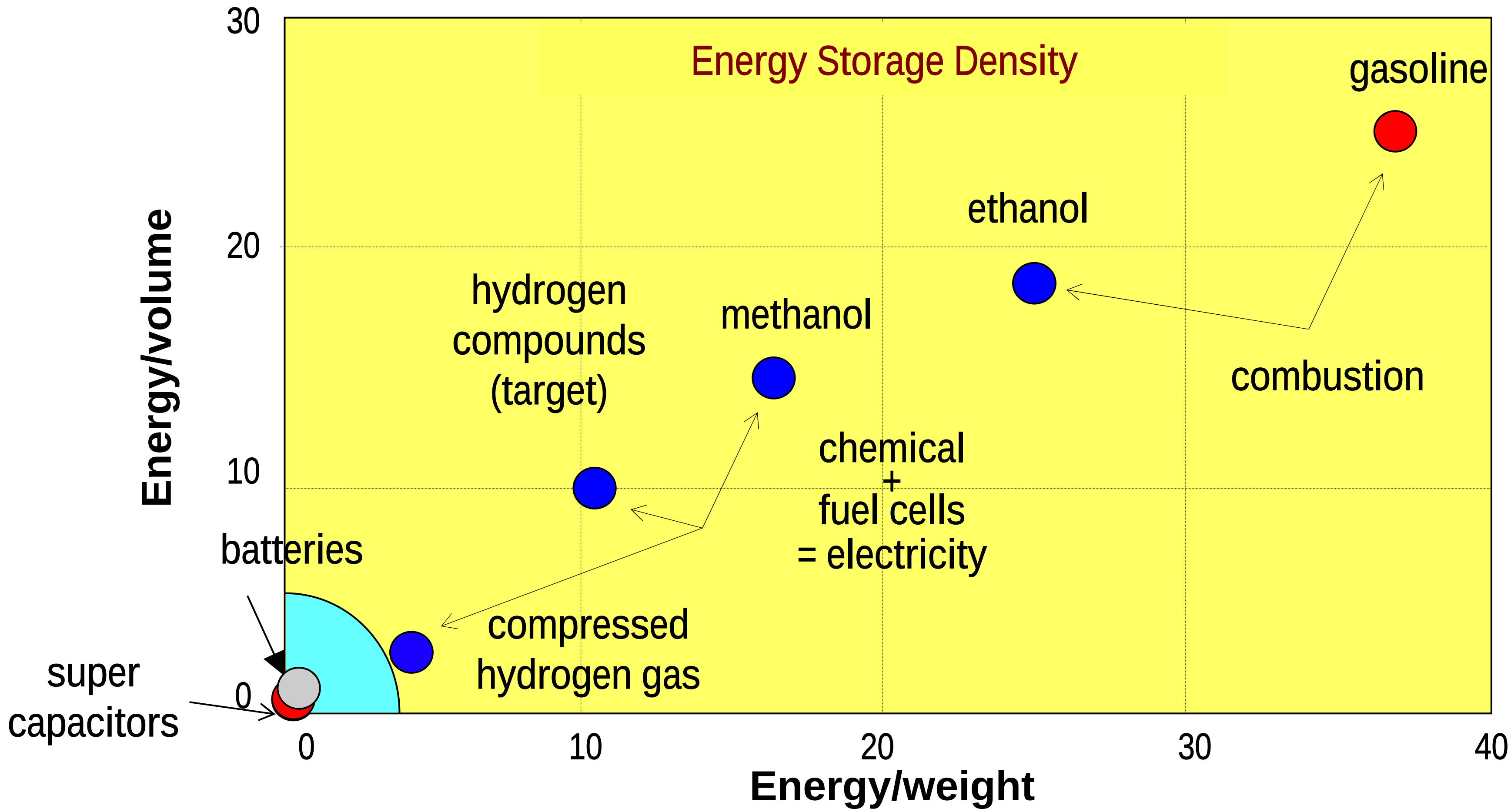
Solar Energy Utilization: Breakthroughs Needed



PV grid parity (~$0.10/kWh) is projected by 2015. But this is not good enough for massive use of solar power. That would require solar at $0.02/kWh (cost of coal). And that bold goal requires basic research and resultant disruptive technology.

Enabling Technologies: Storing Energy

- Store intermittent solar and wind electricity
- Electrify transportation with plug-in hybrids and electric cars



x2-5 increase in battery energy density;
x10-20 increase through chemical storage + fuel cells

DOE's Priorities and Goals Address Diverse Energy and National Needs

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

- Organize and focus on breakthrough science
- Develop and nurture science and engineering talent
- Coordinate DOE work across the department, across the government, and globally

Priority: Change the landscape of energy demand and supply

- Drive energy efficiency to decrease energy use in homes, industry and transportation
- Develop and deploy clean, safe, low carbon energy supplies
- Enhance DOE's application areas through collaboration with its strengths in Science

Priority: Economic Prosperity: Create millions of green jobs and increase competitiveness

- Reduce energy demand
- Deploy cost-effective low-carbon clean energy technologies at scale
- Promote the development of an efficient, "smart" electricity transmission and distribution network
- Enable responsible domestic production of oil and natural gas
- Create a green workforce

Priority: National Security and Legacy: Maintain nuclear deterrent and prevent proliferation

- Strengthen non-proliferation and arms control activities
- Ensure that the U.S. weapons stockpile remains safe, secure, and reliable without nuclear testing
- Complete legacy environmental clean-up

Priority: Climate Change: Position U.S. to lead on climate change policy, technology, and science

- Provide science and technology inputs needed for global climate negotiations
- Develop and deploy technology solutions domestically and globally
- Advance climate science to better understand the human impact on the global environment

Priority: Science and Discovery

Invest in science to achieve transformational discoveries

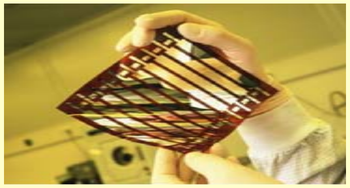
- **Focus on transformational science**
  - Connect basic and applied sciences
  - Re-energize the national labs as centers of great science and innovation
  - Double the Office of Science budget
  - Embrace a degree of risk-taking in research
  - Create an effective mechanism to integrate national laboratory, university, 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

Basic Materials Science and Engineering R&D

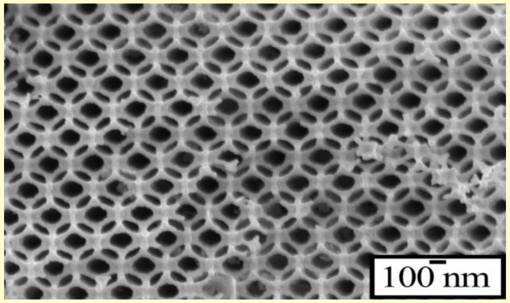
Goal: Achieve a paradigm shift for deterministic design and discovery of new materials with novel structures, functions, and properties

- **Explore the origin of material behaviors**
- **Elucidate fundamental connections to atomic, molecular, and electronic structures**
  - Probe, understand, and control the interactions of photons, electrons, and ions with matter to direct and control energy flow in materials systems over multiple time and length scales
  - Conceptualize, calculate, and predict processes underlying physical transformations and functionality in materials with many atomic constituents, with complex architectures or defects emphasizing emergent behavior
  - Develop experimental techniques and theories/models to understand the behaviors of materials, especially their reactivity under the full range of conditions from near to from equilibrium
  - Explores the interface between physical and biological sciences to assess bio-mimetic processes as new approaches to novel materials design

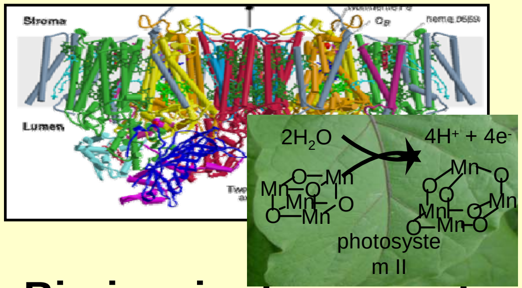
Materials Discovery, Design and Synthesis



Organic and quantum dot-based PV cells



Modified Thermal Emission via Self-Assembly



Bio-inspired nanoscale assemblies: self-repairing and defect-tolerant

Materials Discovery, Design, Synthesis focuses on the science underpinning materials synthesis and control of structure and properties

- **Materials Chemistry**
- **Synthesis and Processing Science:** Development of innovative techniques and understanding via *in situ* monitoring and diagnostic techniques
- **Biomolecular Materials**

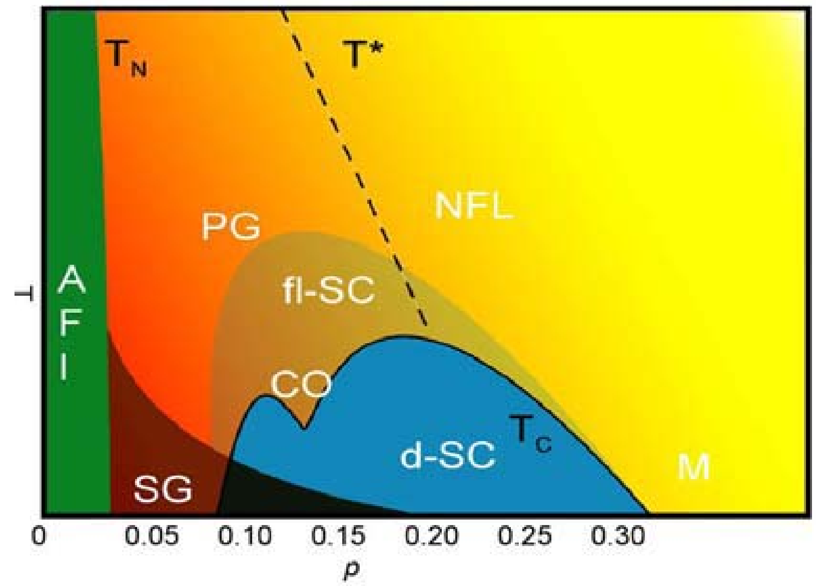
Major thrust areas

- Nanoscale chemical synthesis and assembly of nanomaterials into macroscopic structures
- Solid state chemistry--new classes of superconductors, magnets, thermoelectrics, ferroelectrics
- Surface and interfacial chemistry--electro-catalysis, molecular level understanding of friction, adhesion, lubrication
- Material synthesis and processing science: crystal growth, thin films, multilayer structures, polymers, polymer composites
- Biomimetic/bioinspired materials design and synthesis
- Materials aspects of energy production, conversion and storage based on principles and concepts of biology

Condensed Matter and Materials Physics

Condensed Matter and Materials Physics focuses on the control and understanding of materials and the discovery of new phenomena

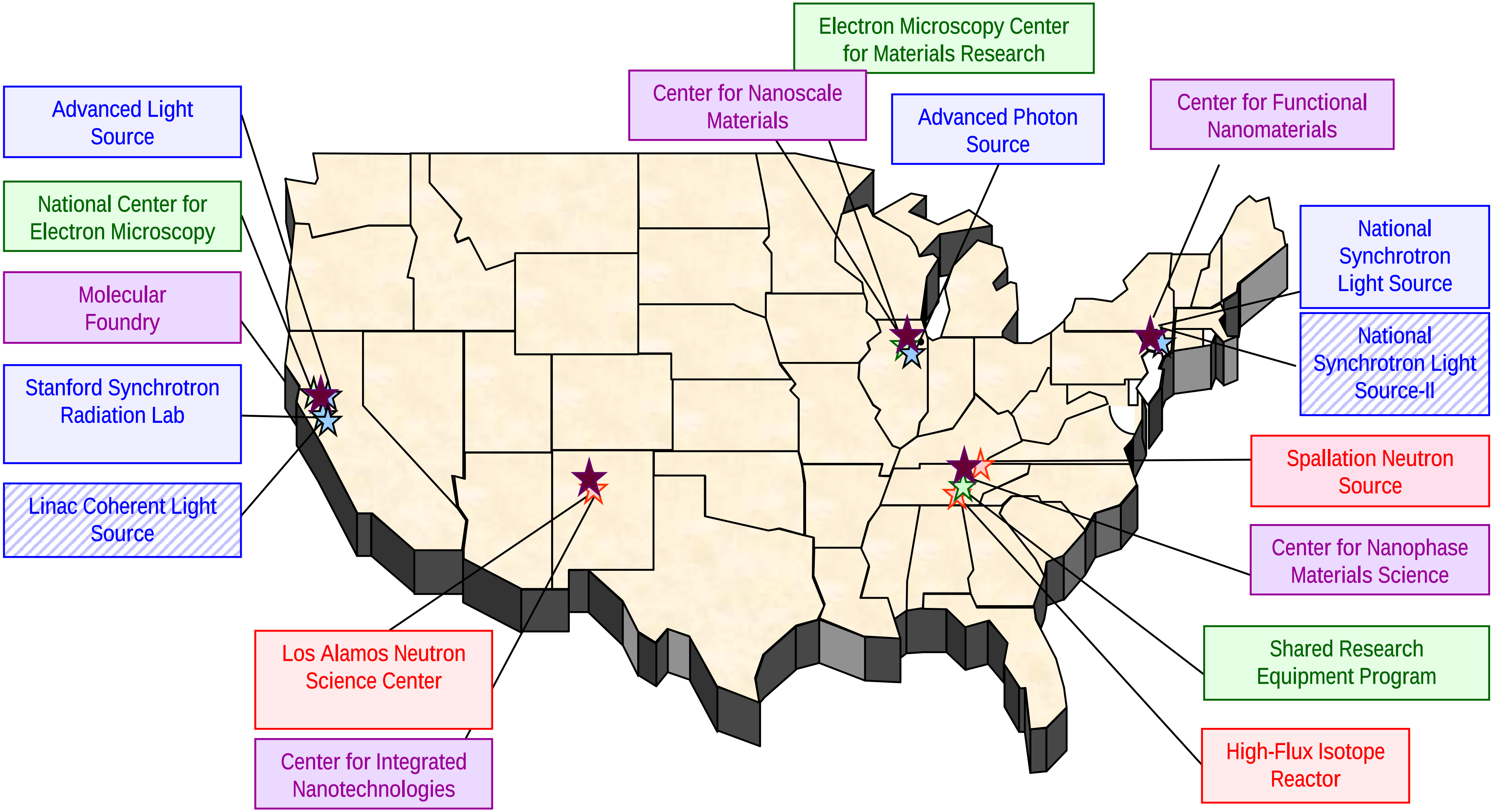
Experimental and Theoretical Condensed Matter Physics
Physical Behavior
Mechanical Behavior and Radiation Effects



Major thrust areas

- Studies of structural, mechanical, electrical, magnetic and optical properties
- Development of predictive models for design of new materials with targeted properties emphasizing control of defect structures that originate from both intrinsic and extrinsic effects.
- Understanding materials' response to variations in temperature, stress, electrical and magnetic fields, chemical and electrochemical environment, and proximity to surfaces or interfaces
- Cooperative and correlation effects that lead to the formation of new particles, new phases of matter and unexpected phenomena

BES Scientific User Facilities: Resources for Materials 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

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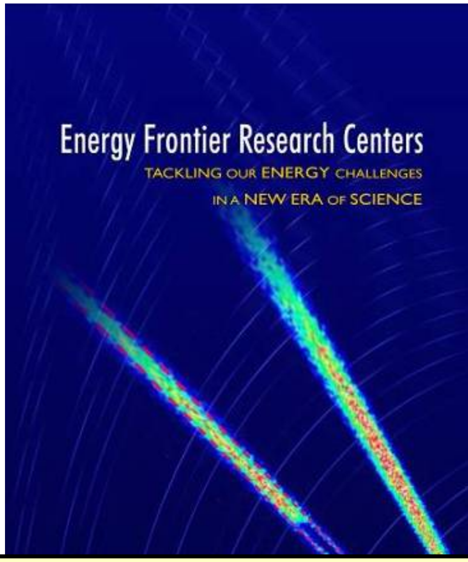
New Strategies for Energy Research: Energy Frontier Research Centers



$100M in the FY 2009 appropriation; $277M in the FY 2009 "Recovery Act;" for a total investment of $777M over a five-year period.

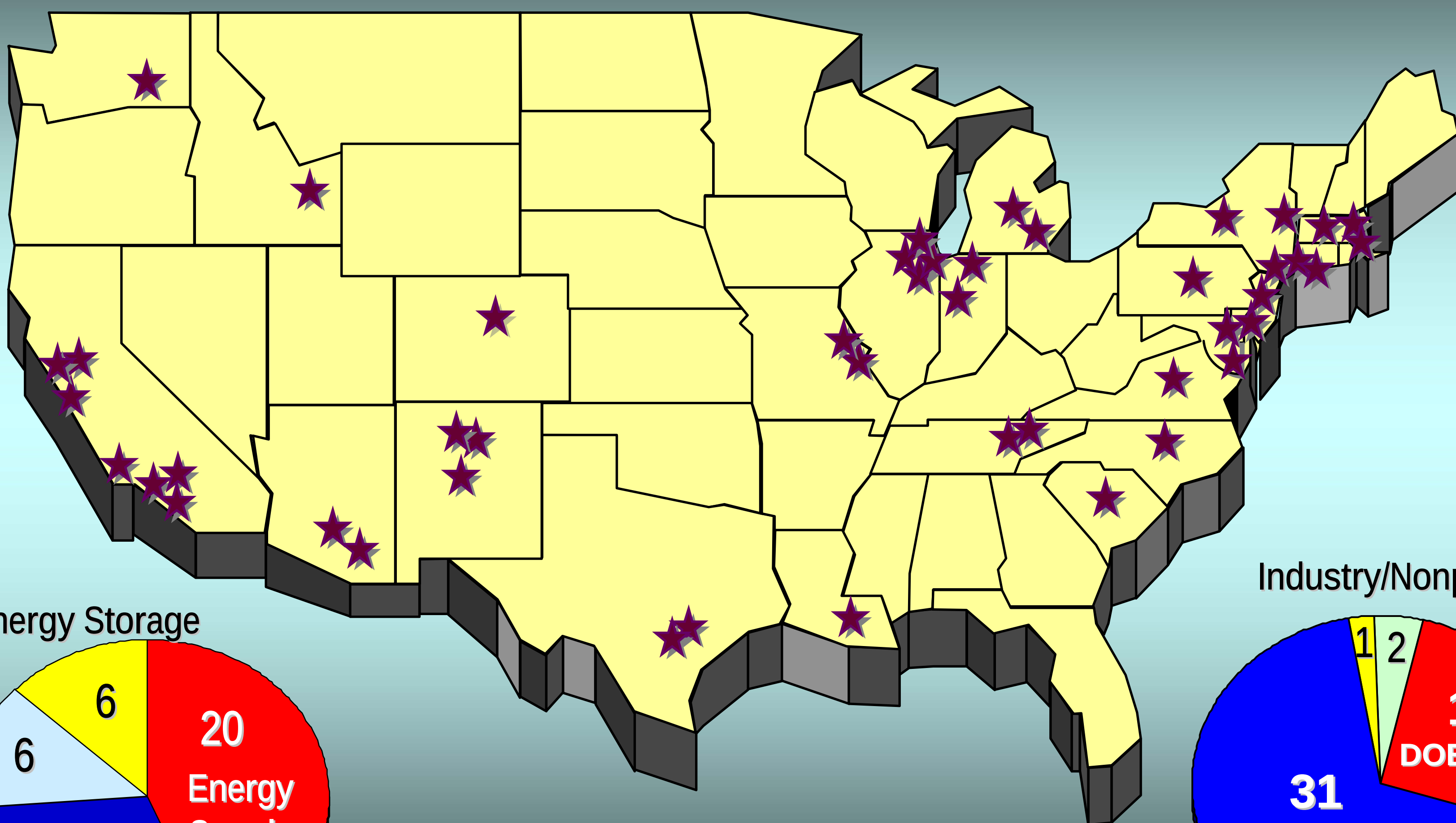
EFRCs will pursue *collaborative* fundamental research that addresses both energy challenges and science grand challenges in:

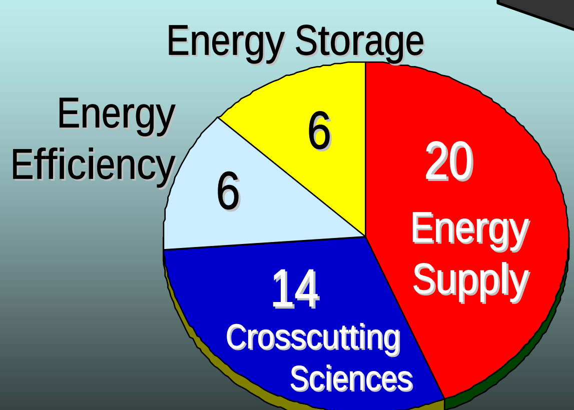
- Solar Energy Utilization
- Catalysis for Energy
- Electrical Energy Storage
- Solid State Lighting
- Superconductivity
- Other
- Geosciences for Nuclear Waste and CO_2 Storage
- Advanced Nuclear Energy Systems
- Combustion of 21st Century Transportation Fuels
- Hydrogen Production, Storage, and Use
- Materials Under Extreme Environments
- Conversion of Biological Feedstock to Portable Fuels

Energy Frontier Research Centers ($2M to $5M/year)

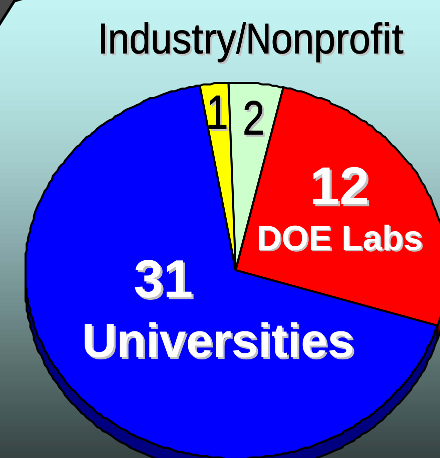
Invest in Cutting-edge Scientific Research to Achieve Transformational Discoveries

46 centers awarded in FY 2009 for five years
Representing 110 participating institutions in 36 states plus D.C.





By Topical Category



By Lead Institution

Solar Energy Utilization: Solar Electricity

Neal R. Armstrong, Univ. of Arizona

Center for Interface Science: Hybrid Solar-Electric Materials –Solar energy to electricity conversion using hybrid inorganic-organic materials focusing on interfacial chemistry.

http://uanews.org/node/25487

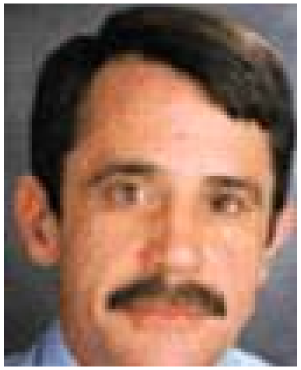
Victor Klimov, LANL

The Center for Advanced Solar Photophysics – Nanoparticle interactions with light to design materials for solar electricity conversion.

James Yardley, Columbia Univ.

Re-Defining Photovoltaic Efficiency Through Molecule-Scale Control – Understand the conversion of sunlight into electricity in nano particles and thin films in organic molecular systems.

http://news.columbia.edu/research/1531



Tom Russell, Univ. of Massachusetts

Polymer-Based Materials for Harvesting Solar Energy -- Use novel, self-assembled polymer materials for the conversion of sunlight into electricity.

http://www.umass.edu/newsoffice/storyarchive/articles/88319.php

Marc Baldo, MIT

Center for Excitonics -- Understand the transport of charge carriers in synthetic disordered systems for conversion of solar energy to electricity and electrical energy storage.

http://web.mit.edu/newsoffice/2009/efrc-0427.html

Solar Energy Utilization: Solar Electricity

Peter Green, Univ of Michigan

Solar Energy Conversion in Complex Materials -- Identify key features in complex materials to design the next generation solar conversion systems. http://www.ns.umich.edu/htdocs/releases/story.php?id=7121

Alex Zunger, NREL

Center for Inverse Design -- Materials for solar energy conversion with an inverse design approach powered by theory and computation.

Donald Morelli, Michigan St. Univ.

Revolutionary Materials for Solid State Energy Conversion -- Understand physical and chemical principles of advanced materials for the conversion of heat into electricity.

http://news.msu.edu/story/6271/

Gang Chen, MIT

Solid-State Solar-thermal Energy Conversion Center -- Create novel, solid-state materials for the conversion of sunlight and heat into electricity.

http://web.mit.edu/newsoffice/2009/efrc-0427.html

Solar Energy Utilization: Solar Fuels

Robert Blankenship, Washington Univ., St. Louis MO

Photosynthetic Antenna Research Center -- Understand photosynthetic antenna system to convert sunlight into fuels.

http://news-info.wustl.edu/news/page/normal/14079.html

Tom Meyer, Univ. of North Carolina

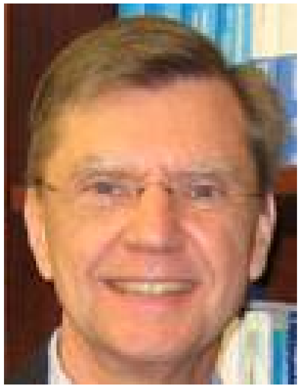
Solar Fuels and Next Generation Photovoltaics -- Nanoscale architectures for improved generation of fuels and electricity from sunlight.

http://uncnews.unc.edu/news/science-and-technology/unc-to-launch-solar-fuels-research-center-with-17.5-million-in-federal-energy-stimulus-grant.html

Devens Gust, Arizona St. Univ.

Bio-Inspired Solar Fuel Production - Adapt natural photosynthesis principles to bio-inspired approaches for solar fuels production.

http://asunews.asu.edu/20090430_EFRC



Michael Wasielewski, Northwestern Univ.

Argonne-Northwestern Solar Energy Research Center -- Revolutionize the design, synthesis, and control of molecules for solar fuels generation.

http://www.northwestern.edu/newscenter/stories/2009/04/efrc.html

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Bio-Fuels

Richard Sayre, Donald Danforth Plant Science Center

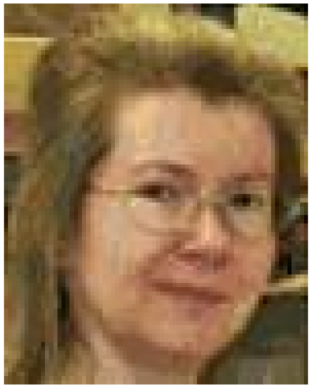
Center for Advanced Biofuels Systems -- Photosynthesis and production of energy-rich molecules in plants.

http://www.danforthcenter.org/newsmedia/NewsDetail.asp?nid=164

Maureen McCann, Purdue Univ.

Center for Direct Catalytic Conversion of Biomass to Biofuels -- Conversion mechanism of biomass to fuels or chemicals.

http://www.science.purdue.edu/



Daniel Cosgrove, Penn St. Univ.

Center for Lignocellulose Structure and Formation – Physical structure of bio-polymers in plant cell walls for converting biomass into fuels.

http://casey.senate.gov/newsroom/press/release/?id=d6e10a4d-9eb2-4a85-8c1f-f7d76176488d

Energy Storage

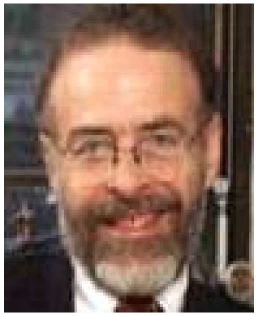
Michael Thackeray, ANL

Center for Electrical Energy Storage -- Understand complex phenomena in electrochemical reactions critical to advanced electrical energy storage.

http://www.anl.gov/Media_Center/News/2009/news090428.html

Grigorii Soloveichik, General Electric Global Research

Center for Innovative Energy Storage -- Explore the fundamental chemistry of electrocatalysis and ionic transport for energy storage that combines the best properties of a fuel cell and a flow battery.



Héctor Abruña, Cornell Univ.

Nanostructured Interfaces for Energy Generation, Conversion, and Storage -- Understand the nature, structure, and dynamics of reactions at electrodes.

http://www.news.cornell.edu/stories/May09/EFRC.ws.html

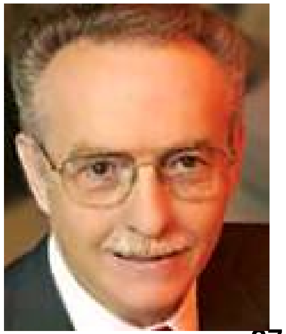
Clare P. Grey, Stony Brook Univ.

Northeastern Chemical Energy Storage Center -- Overcoming performance barriers of batteries through electrode designs.

http://commcgi.cc.stonybrook.edu/am2/publish/Research_20/DOE_to_Establish_Energy_Frontier_Research_Center_at_Stony_Brook_University.shtml

Gary Rubloff, Univ. of Maryland

Science of Precision Multifunctional Nanostructures for Electrical Energy Storage -- Understand and build nano-structured electrode components.



Ken Reifsnider, Univ. of South Carolina

Nano-Structure Design and Synthesis of Heterogeneous Functional Materials – Focusing on nano-structured materials functions at interfaces

http://www.sc.edu/news/newsarticle.php?nid=175

Energy Efficiency

Jerry Simmons, SNL

Solid State Lighting Science -- Understand energy conversion in tailored nanostructures for solid-state lighting.

http://www.sandia.gov/news/resources/releases/2009/energy-frontier.html

John Bowers, UCSB

Center on Materials for Energy Efficiency Applications -- Discover and develop materials that control the interactions between light, electricity, and heat at the nanoscale.

http://engineering.ucsb.edu/news/249

Harry Atwater, Caltech

Light-Material Interactions in Energy Conversion -- Tailor the properties of advanced materials to control the flow of solar energy and heat.

http://today.caltech.edu/today/story-display?story_id=36162

Daniel Dapkus, Univ. of Southern California

Emerging Materials for Solar Energy Conversion and Solid State Lighting -- Hybrid inorganic-organic materials for solar energy conversion and solid state lighting.

http://viterbi.usc.edu/news/news/2009/dapkus-wins-12.htm

Séamus Davis, BNL

Center for Emergent Superconductivity -- Understand the fundamental physics of superconductivity for electricity transmission and grid-related applications.

http://www.bnl.gov/bnlweb/pubaf/pr/PR_display.asp?prID=953

Chung Law, Princeton Univ.

Combustion Science -- Develop predictive combustion modeling capabilities for design and utilization of non-petroleum based fuels in transportation.

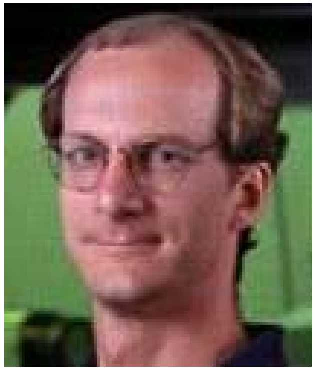
http://www.princeton.edu/main/news/archive/S24/15/38M61/index.xml?section=topstories

Advanced Nuclear Energy Systems

Dieter Wolf, Idaho National Lab

Center for Materials Science of Nuclear Fuel – Understand radiation-resistant and mechanical behavior of advanced nuclear fuel materials.

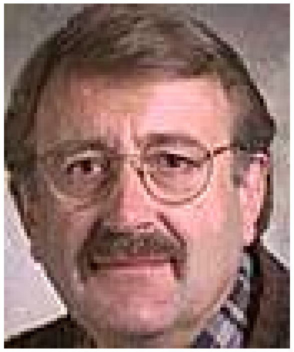
https://inlportal.inl.gov/portal/server.pt?open=514&objID=1555&mode=2&featurestory=DA_312358



Peter Burns, Univ. of Notre Dame

Materials Science of Actinides – Understand physical and chemical behavior of nanoscale actinides-containing materials in extreme environments for advance nuclear energy systems.

http://newsinfo.nd.edu/news/11640-doe-to-establish-energy-frontier-research-center-at-notre-dame



Malcolm Stocks, ORNL

Energy Frontier Center for Defect Physics in Structural Materials -- Understand the interactions and dynamics of defects in alloys under extreme radiation environments.

http://www.ornl.gov/ornlhome/print/press_release_print.cfm?ReleaseNumber=mr20090428-00

Michael Nastasi, LANL

Extreme Environment-Tolerant Materials via Atomic Scale Design of Interfaces – Understand the behavior of materials subject to extreme radiation doses and mechanical stress.

Carbon Capture and Management

Gary Pope, Univ. of Texas, Austin

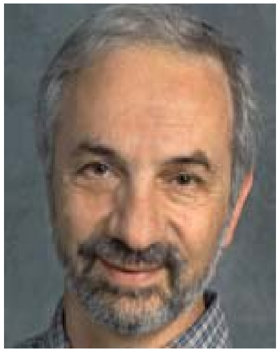
Frontiers of Subsurface Energy Security -- Understand the transport of CO2 in geological systems over multiple length scales.

http://www.utexas.edu/news/2009/04/29/solar_cells_batteries/

Berend Smit, UC-Berkeley

Center for Gas Separations Relevant to Clean Energy Technologies -- Design and synthesize new matter with tailored properties for carbon capture and sequestration.

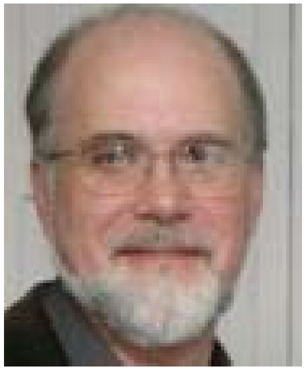
http://chemistry.berkeley.edu/publications/news/2009/smit_head_energy_frontiers_research_center.html



Donald DePaolo, LBNL

Center for Nanoscale Control of Geologic CO2 -- Establish the scientific foundations for the CO2 storage.

http://newscenter.lbl.gov/feature-stories/2009/04/28/efrc-co2/



David Wesolowski, ORNL

Fluid Interface Reactions, Structures and Transport Center -- Provide basic scientific understanding of phenomena that occur at interfaces in energy systems.

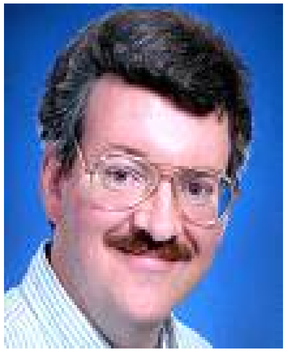
http://www.ornl.gov/ornlhome/print/press_release_print.cfm?ReleaseNumber=mr20090428-00

Catalysis for Energy Applications

Brent Gunnoe, Univ. of Virginia

Center for Catalytic Hydrocarbon Functionalization -- Novel catalysts for the efficient conversion of hydrocarbon gases into liquid fuels.

http://www.virginia.edu/uvatoday/newsRelease.php?id=8539#



Morris Bullock, PNNL

Center for Molecular Electrocatalysis -- Understand the chemical and electrical energy exchange mechanisms in electrocatalytic processes involving multi-protons and multi-electron redox reactions.

http://www.pnl.gov/news/release.asp?id=367

Dion Vlachos, Univ. of Delaware

Rational Design of Innovative Catalytic Technologies for Biomass Derivative Utilization -- Catalysts for converting biomass into chemicals and fuels.

http://www.udel.edu/udaily/2009/may/efrc050409.html

Jerry Spivey, Louisiana St. Univ.

Computational Catalysis and Atomic-Level Synthesis of Materials -- Develop computational tools to model catalytic reactions and to design of new catalysts.

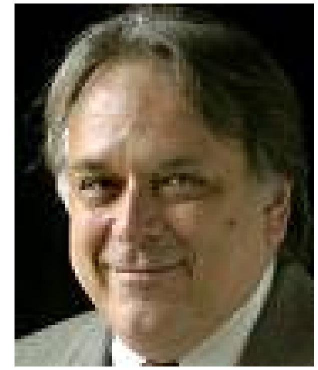
http://appl003.lsu.edu/unv002.nsf/9faf000d8eb58d4986256abe00720a51/a154b03fa22d1135862575a9004f34a6?OpenDocument

Chris Marshall, ANL

Institute for Atom-Efficient Chemical Transformations – Understand chemical mechanisms to extend the utilization of coal and biomass.

http://www.anl.gov/Media_Center/News/2009/news090428.html

Advanced Energy Materials



Paul Barbara, Univ. of Texas, Austin

Charge Separation and Transfer at Interfaces in Energy Materials and Devices -- Understand charge transfer processes of molecular materials.

http://www.utexas.edu/news/2009/04/29/solar_cells_batteries/

Vidvuds Ozolins, UCLA

Molecularly Assembled Material Architectures for Solar Energy Production, Storage, and Carbon Capture

http://www.newsroom.ucla.edu/portal/ucla/new-multi-million-dollar-energy-90536.aspx

Bartosz Grzybowski, Northwestern Univ.

Center for Far-From-Equilibrium and Adaptive Materials -- Understand new classes of materials under conditions far from equilibrium for energy applications.

http://www.northwestern.edu/newscenter/stories/2009/04/efrc.html

David Mao, Carnegie Institute of Washington

Center for Energy Frontier Research in Extreme Environments -- Materials that can tolerate transient extremes in pressure and temperature.

http://www.ciw.edu/news/carnegie_wins_doe_energy_frontier_research_center_award

Fritz Prinz, Stanford Univ.

Center on Nanostructuring for Efficient Energy Conversion -- Design, create, and characterize materials at the nanoscale for a wide variety of energy applications.

http://news.stanford.edu/news/2009/may13/nanotech-051309.html

U.S. DEPARTMENT OF ENERGY

Single-Investigator and Small-Group Research

Tackling our energy challenges in a new era of science

- In FY 2009 $55M will be available for single-investigator and small-group awards.
- BES sought applications in two areas: grand challenge science and energy challenges identified in one of the Basic Research Needs workshop reports.
- Awards are planned for three years, with funding in the range of $150-300k/yr for single-investigator awards and $500-1500k/yr for small-group awards (except as noted below)
- Areas of interest include:

  Grand challenge science: ultrafast science; chemical imaging, complex & emergent behavior

  Tools for grand challenge science: midscale instrumentation; accelerator and detector research (awards capped at $5M over 3-year project duration)

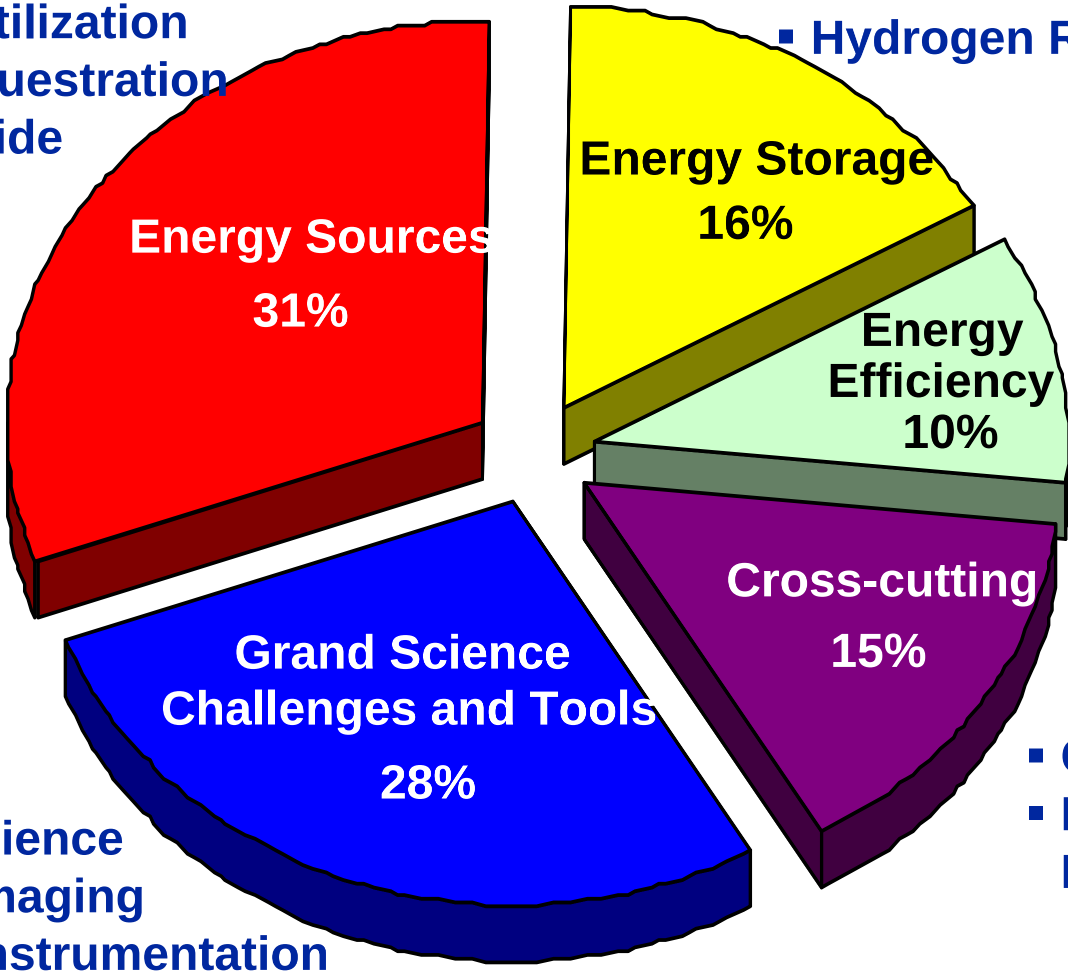
  Use inspired discovery science: basic research for electrical energy storage; advanced nuclear energy systems; combustion of 21st century fuels; hydrogen production, storage, and use; other basic research areas identified in BESAC and BES workshop reports with an emphasis on nanoscale phenomena
- Full proposals were due April 24, 2009 and decisions will be made soon
- For full details see: http://www.sc.doe.gov/bes/SISGR.html

SISGR Solicitation: 879 White Papers

~ 88% from Universities; 11% DOE Labs; 1% Other Institutions

- Advanced Nuclear Energy Systems
- Solar Energy Utilization
- Geological Sequestration of Carbon Dioxide

- Electrical Energy Storage
- Hydrogen Research



- Solid-state Lighting
- Clean and Efficient Combustion
- Superconductivity

- Catalysis for Energy
- Materials under Extreme Environments

- Ultrafast Science
- Chemical Imaging
- Mid-scale Instrumentation
- Complex Systems and Emergent Behavior

Basic Energy Sciences (BES)

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BES Mission: To support fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels in order to provide the foundations for new energy technologies and to support DOE missions in energy, environment, and national security.

Priorities:

- Create a new paradigm for the design of materials, especially those related to the efficient production, storage, transmission, and use of energy
- Through observation and manipulation of matter at atomic and molecular scales, achieve mastery of material syntheses and chemical transformations relevant to real-world energy systems
- Understand and control fundamental interactions between matter and energy, especially at the nanoscale
- Conceive, construct, and operate open-access scientific user facilities to probe materials at the limits of time, space, and energy resolution

Program Planning Factors for FY 2010:

- Significant effort will be spent in establishing the EFRCs and in overseeing new facilities (LCLS) and a major construction project (NSLS-II).
- Efforts in FY 2010 are informed by the previous Scientific Workshops and Reports: BESAC *Basic Research Needs* workshop series (11 workshops from 2003-2007); BESAC *Energy Grand Challenges* report (2007); BESAC *New Science for a Secure and Sustainable Energy Future* (2008)
- **R&D coordination with DOE applied technology programs in areas such as electrical energy storage, solar energy utilization, biofuels, and fuel cells**
- 2009 Recovery Act enhancements

BES FY 2010 Highlights

Research (3 modalities):

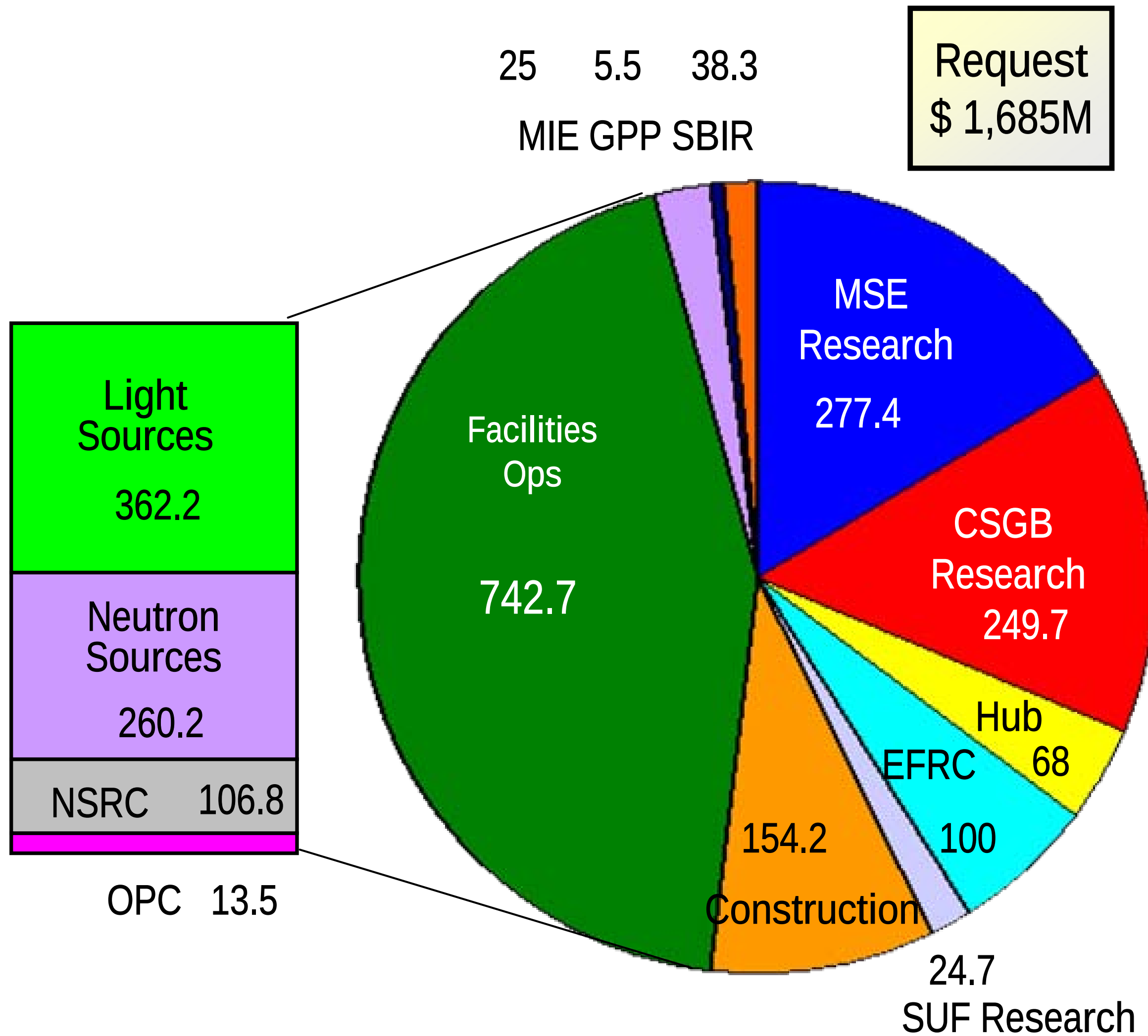
- **Core research** supporting single investigators and small groups is continued. This includes research addressing the 5 key science challenges from the BESAC Grand Challenges report: (1) quantum control of electrons in atoms, molecules, and materials; (2) basic atomic architecture of matter and directed assembly; (3) emergence and collective phenomena; (4) energy and information transfer on the nanoscale; and (5) matter far from equilibrium.
- **Energy Frontier Research Centers (EFRCs)**, initiated late in FY 2009, see their first full year of operation in FY 2010. The 46 new EFRCs assemble scientists from multiple disciplines to conduct basic research to establish the scientific foundations for new energy technologies in a wide variety of topical areas.
- **Energy Innovation Hubs** are initiated in the areas of **Fuels from Sunlight** and **Batteries and Energy Storage**. Hubs assemble purpose-driven teams to address the basic science, technology, economic, and policy issues needed to address the energy topic. Each is funded at $25,000,000/year for an initial 5 year-period with one-time funding of $10,000,000 provided for start-up, excluding new construction.

Facilities:

- **Scientific User Facility Operations** are fully funded in FY 2010. More than 10,000 scientists and engineers from academia, national laboratories, and industry use the BES facilities annually.
- The **Linac Coherent Light Source (LCLS)** at SLAC National Accelerator Laboratory, the world's first hard x-ray coherent light source, begins operations in FY 2010. First science starts in the fall of 2009.
- The **National Synchrotron Light Source II** at Brookhaven National Laboratory continues construction, including the largest component of the project—the building that will house the storage ring.

FY 2010 BES Budget Request

- **Core research programs**
  - 2 Energy Innovation Hubs at $25M plus ~$10M start-up
  - $100M for Energy Frontier Research Centers
  - Core research increases for grand challenge science, accelerator & detector research
- **Scientific user facilities operations**
  - Synchrotron light sources
  - Neutron scattering facilities
  - Nanoscale Science Research Centers
- **Construction and instrumentation**
  - National Synchrotron Light Source-II
  - Linac Coherent Light Source
  - Spallation Neutron Source instruments and Power Upgrade



DOE currently funds 3 Bioenergy Research Centers ($25M/year each)

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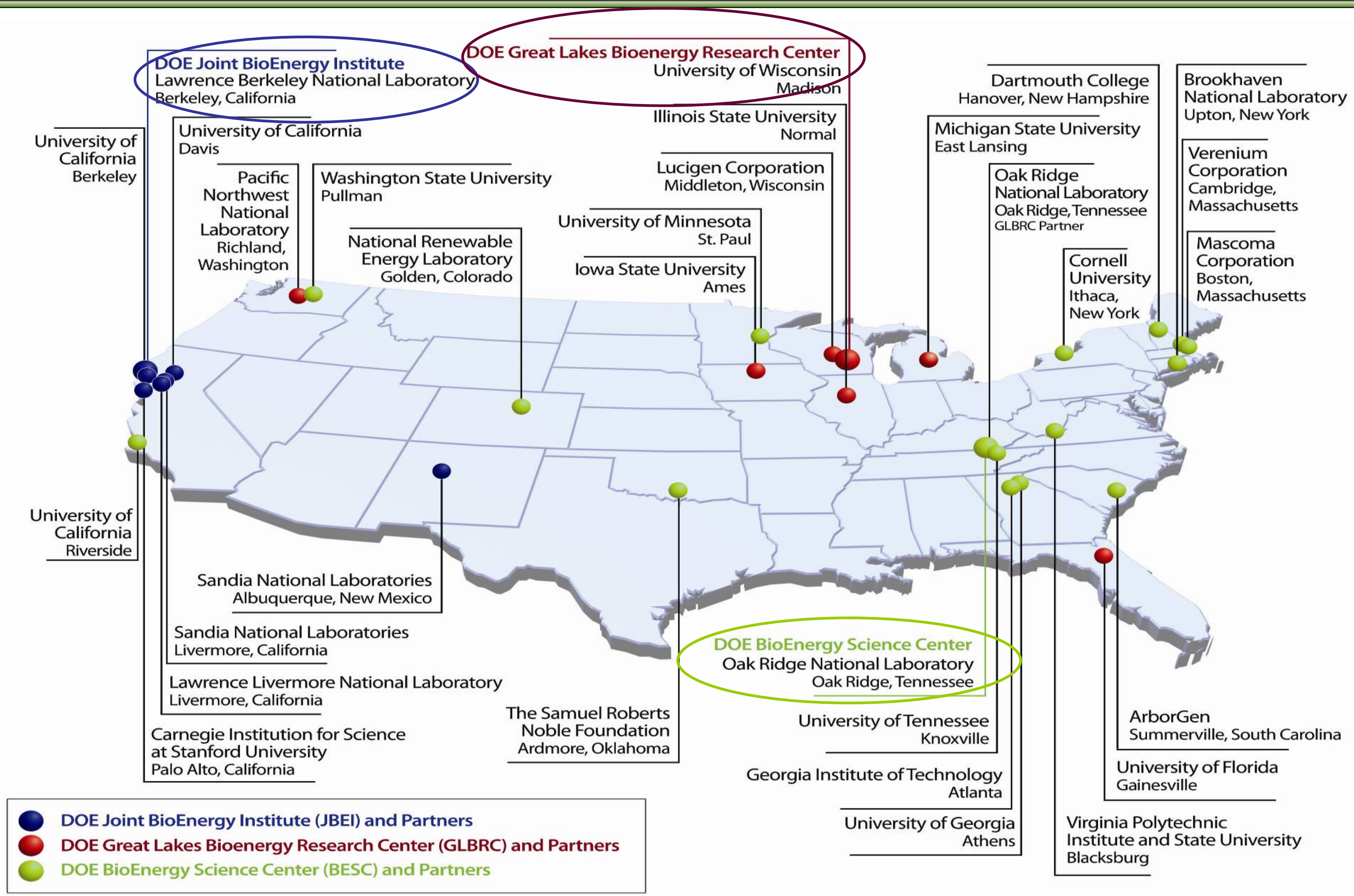

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Proposed DOE Hub Topical Areas

- **Office of Science, BES:**
  - Fuels from Sunlight;
  - Batteries and Energy Storage
- **Energy Efficiency and Renewable Energy:**
  - Solar Electricity;
  - Energy Efficient Building Systems Design
- **Fossil Energy:**
  - Carbon Capture and Storage;
- **Office of Electricity:**
  - Grid Materials, Devices, and Systems;
- **Nuclear Energy:**
  - Extreme Materials;
  - Modeling and Simulation

Some Program Features

(Source: Pat Dehmer, May 20, 2009, presentation to Energy Sciences Coalition)

	Investigators and their institutions	Central location for investigators?	Diversity of Disciplines	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. The model is the three existing SC Bio-energy Research Centers.	Yes, there is a central location (building) housing many/most of the investigators. A significant aspect of the Hubs is the collocation of researchers. Collaborators at other institutions may partner with the Hub leader. Industries may also be associated with Hubs.	Many	5 years with one 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.	$25M/year with $10M additional in the 1st year for CE or building mods.	Purpose-driven research, spanning fundamental, transformational science to commercialization. The breadth and emphasis of activities will be influenced greatly by the nature of the Hub. For example, the topics of some Hubs are ready for commercialization or improved manufacturing methods (solar photovoltaics). Other Hubs address topics that may require greater emphasis on fundamental research. In general, DOE determines the topical areas of the Hubs, and FOAs are specific.
Energy Frontier Research Centers	Self-assembled group of ~6-12 investigators. May be led by Labs or universities. About 2/3 of EFRCs are led by universities.	Ideally, each EFRC will have a lead institution, home to many/most of the investigators, but there is flexibility.	Several	5 years with 5-year renewals possible. Managed by SC/BES	$2-5M/year	Fundamental, transformational research with a clear link to new energy energy technologies or technology roadblocks. In general, the investigators propose the subject matter from among a large set of general energy-relevant topics, and FOAs are broad.
ARPA-E	Single investigator, small group, or small teams.	No	Few	1-3 years Managed by ARPA-E, which reports to the Secretary of Energy	$0.5 - 10M/year	High risk research driven by the potential for significant commercial impact. In general, DOE determines the area of interest.

"How Nature Works" to "Materials and Processes by Design" to "Technologies for the 21st Century"

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Grand Challenges *How nature works*	Discovery and Use-Inspired Basic Research *Materials properties and functionalities by design*		Applied Research	Technology Maturation & Deployment

Grand Challenges

- **Controlling materials processes at the level of quantum behavior of electrons**
- **Atom- and energy-efficient syntheses of new forms of matter with tailored properties**
- **Emergent properties from complex correlations of atomic and electronic constituents**
- **Man-made nanoscale objects with capabilities rivaling those of living things**
- **Controlling matter very far away from equilibrium**

Discovery and Use-Inspired Basic Research

- **Basic research for fundamental new understanding on materials or systems that may revolutionize or transform today's energy technologies**
- **Development of new tools, techniques, and facilities, including those for the scattering sciences and for advanced modeling and computation**

- **Basic research, often with the goal of addressing showstoppers on real-world applications in the energy technologies**

Applied Research

- **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**
- **Proof of technology concepts**

Technology Maturation & Deployment

- **Scale-up research**
- **At-scale demonstration**
- **Cost reduction**
- **Prototyping**
- **Manufacturing R&D**
- **Deployment support**

Energy Frontier Research Centers

Single PI and Small Groups Research

DOE Technology Office/Industry Roadmaps

Questions?