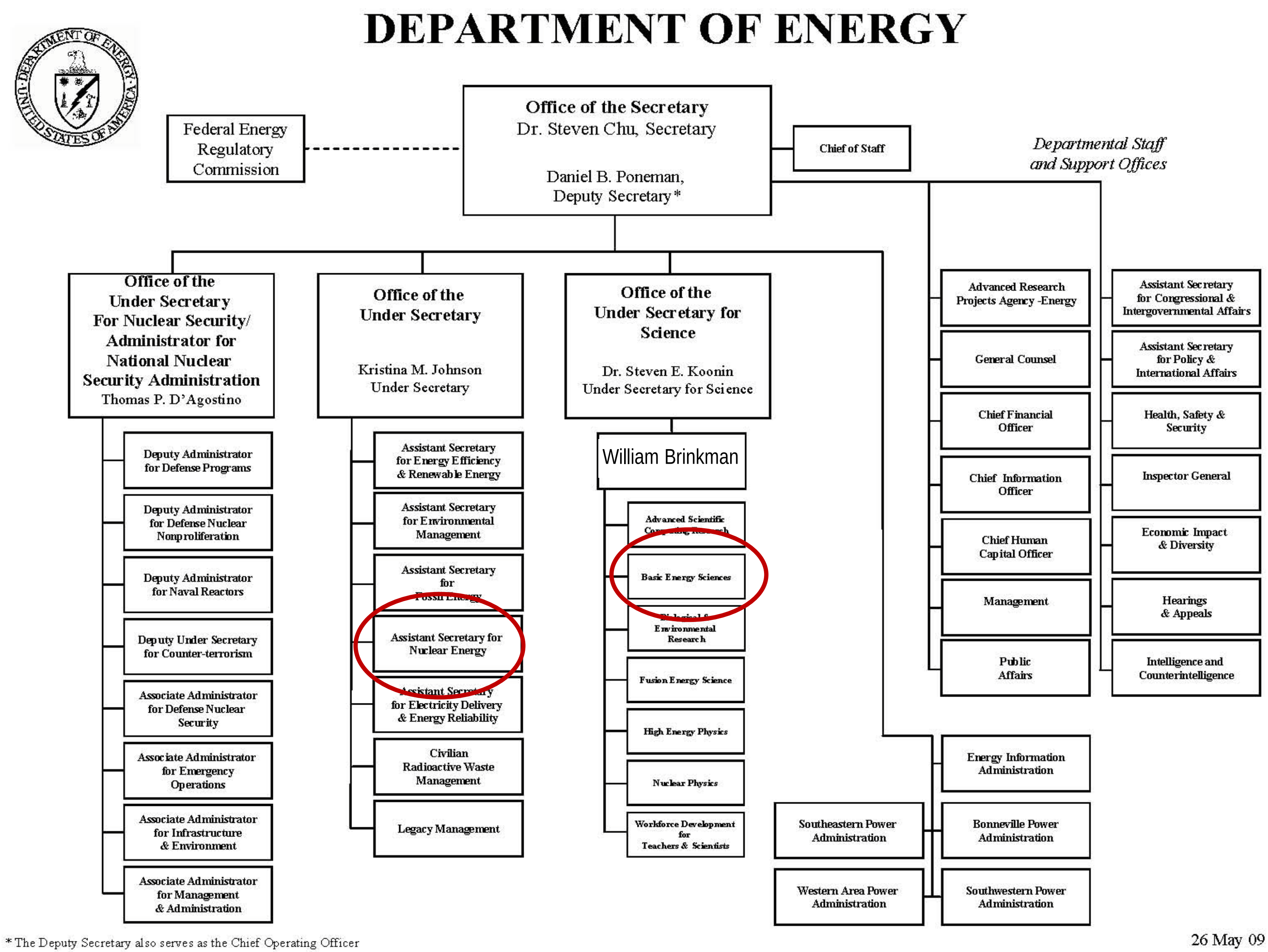
U.S. DEPARTMENT OF ENERGY | Office of Science

Materials for Extreme Environments: A Perspective from DOE-Basic Energy Sciences

June 15, 2010

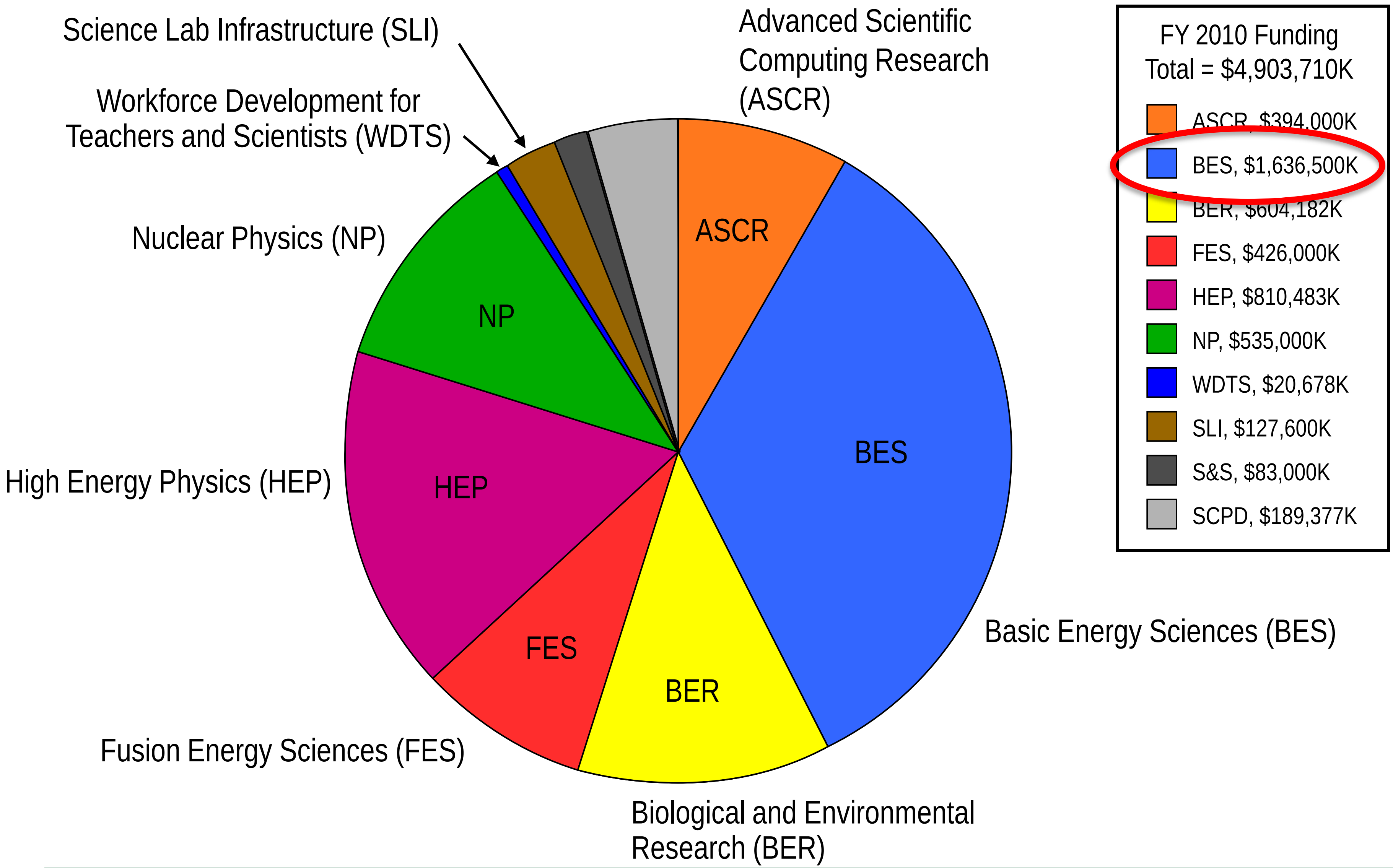
Linda Horton
Division of Materials Sciences and Engineering
Office of Basic Energy Sciences, Office of Science
U.S. Department of Energy

DOE – From Fundamental Science to Technology Research



Office of Science Programs

FY 2010 Appropriation



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
- Robin Hayes, AAAS Fellow
- Katie Perine, Program Analyst / BESAC
- Ken Rivera, Laboratory Infrastructure / ES&H
- Vacant, DOE and Stakeholder Interactions

Materials Sciences and Engineering Division

Linda Horton, Director

Vacant, Program Analyst
Charnice Waters, Secretary

Materials Discovery, Design, and Synthesis
Arvind Kini
Kerry Gorey, P.A.

- **Materials Chemistry** — Mary Galvin; Dick Kelley; ● Darryl Sasaki, SNL
- **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; Jim Horwitz; ◆ 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; Jane Zhu; ● Helen Farrell, INL; ● John Schlueter, ANL

* 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; Peter Lee
- **NSRCs and EBMCs**** — Tof Carim; Carlos Sa de Melo; ◆ Joe Horton, ORNL
- **Accelerator and Detector R&D** — Eliane Lessner
- **Facility Coordination; Metrics; Assessment** — Van Nguyen

** Nanoscale Science Research Centers and Electron-beam Microcharacterization Centers

Construction
- **Linac Coherent Light Source** — Tom Brown
- **National Synchrotron Light Source II** — Tom Brown
- **Spallation Neutron Source Upgrades** — Tom Brown
- **Instrument MIEs***** — Stephen Tkaczyk; ◆ John Tapia, LANL
- **Advanced Light Source User Support Building** — Tom Brown

*** Major Item of Equipment projects

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

Photochemistry and Biochemistry
Rich Greene
Sharron Watson, P.A.

- **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; ◆ Jan Hrbek, BNL
- **Heavy Element Chemistry** — Vacant; △ Larry Rahn, SNL; ● Norm Edelstein, LBNL
- **Separations and Analysis** — Bill Millman; △ Larry Rahn, SNL
- **Geosciences** — Nick Woodward; ● Jennifer Blank, LBNL
- **Technology Office Coordination** — Marvin Singer; Vacant

LEGEND
- ◆ Detailee (from DOE laboratories)
- ■ Detailee, ½ time, not at HQ
- ● Detailee, ¼ time, not at HQ
- ◆ On detail to EERE/SETP, 30%
- △ IPA (Interagency Personnel Act)
- P.A. Program Assistant

May 2010

Basic Energy Sciences Mission

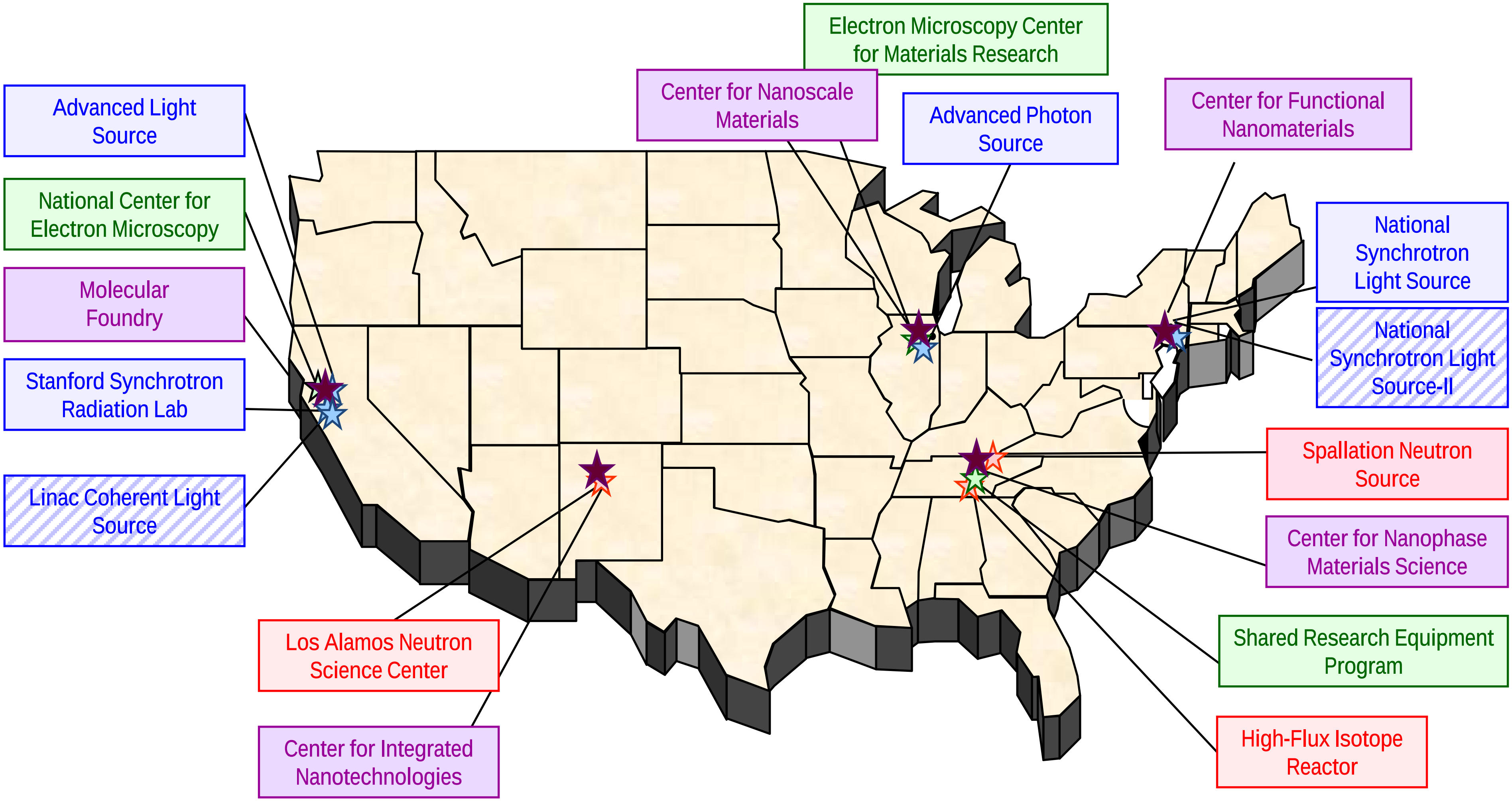
Mission:

- 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:

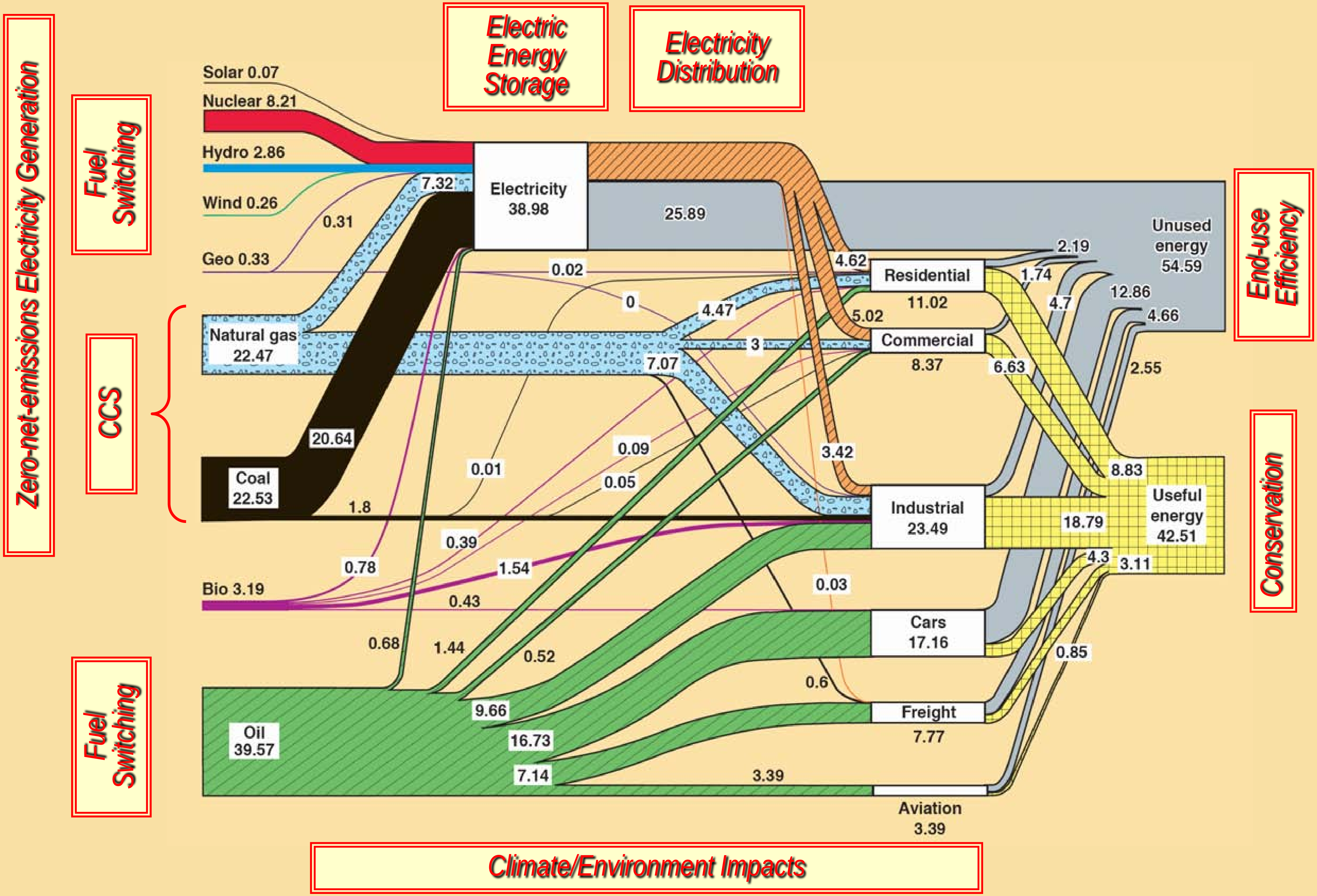
- Discover and design new materials and molecular assemblies with novel function, through atom-by-atom and molecule-by-molecule control
- Conceptualize, calculate, and predict processes underlying physical and chemical transformations
- Probe, understand, and control the interactions of phonons, photons, 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

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

Key R&D Strategies



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

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

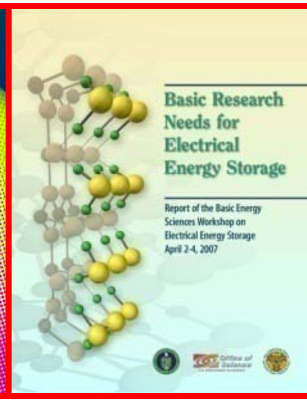
2003 Workshop and Report

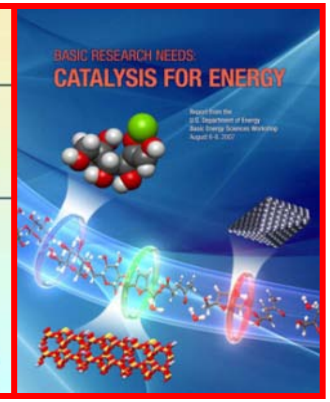
- Indentified broad, basic research directions to support the scientific advances to resolve major energy technological changes
- Series of ten follow-on *Basic Research Needs* workshops
  - >1,500 participants from universities, industry, and federal laboratories
  - In-depth analyses of scientific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

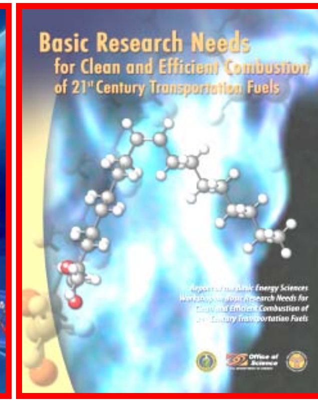
Proposed Research Directions - Basic Research Needs for a Secure Energy Future (2003)

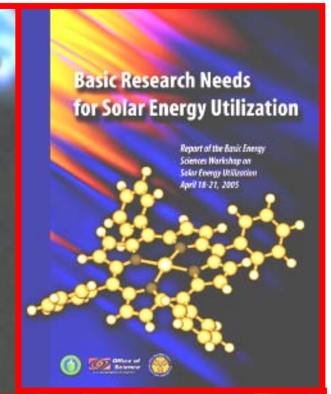
- **Nuclear Fission Energy**
  - Materials Degradation
  - Advanced Actinide and Fission Product Separations and Extraction
  - Fuels Research
  - Fundamental Research in Heat Transfer and Fluid Flow
- **Fusion Energy**
  - Multiscale Modeling of Microstructural Stability of Irradiated Materials
  - Deformation and Fracture Modeling
  - Plasma-Surface Interactions
  - Thermofluids and "Smart Liquids"
  - Plasma Aerodynamics

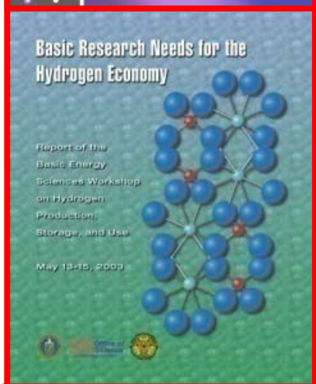
Strategies: Ten "Basic Research Needs …" Workshops











Hydrogen Economy

Solar Energy Utilization

Superconductivity

Solid State Lighting

Advanced Nuclear Energy Systems

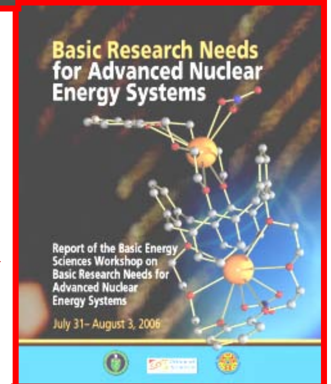
Clean and Efficient Combustion of 21st Century Transportation Fuels

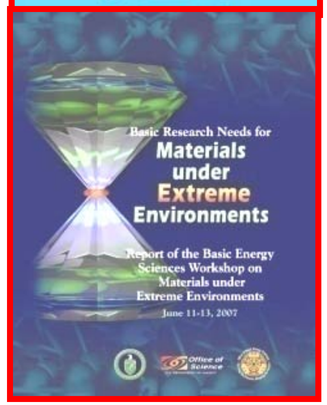
Geosciences: Facilitating 21st Century Energy Systems

Electrical Energy Storage

Catalysis for Energy Applications

Materials under Extreme Environments





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

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

Grand Challenges *How nature works*	Discovery and Use-Inspired Basic Research *Materials properties and functionalities by design*		Applied Research	Technology Maturation & Deployment
▪ 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	▪ 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	▪ Research with the goal of meeting <u>*technical milestones*</u>, with emphasis on the development, performance, cost reduction, and durability of materials and components or on efficient processes ▪ Proof of technology concepts	▪ Scale-up research ▪ At-scale demonstration ▪ Cost reduction ▪ Prototyping ▪ Manufacturing R&D ▪ Deployment support

BESAC & BES Basic Research Needs Workshops

BESAC Grand Challenges Report

DOE Technology Office/Industry Roadmaps

Basic Energy Sciences
Goal: new knowledge / understanding
Mandate: open-ended
Focus: phenomena
Metric: knowledge generation

DOE Technology Offices: EERE, NE, FE, EM, …
Goal: practical targets
Mandate: restricted to target
Focus: performance
Metric: milestone achievement

From Science to Deployment – Overview of the ANES Workshop

Discovery Research	Use-inspired Basic Research	Applied Research	Technology Maturation & Deployment

Discovery Research / Use-inspired Basic Research

- Accurate relativistic electronic structure approaches for correlated f-electron systems
- Integration of multi-physics, multi-scale computational models: atomistic to continuum
- Reactivity, dynamics, molecular speciation and kinetic mechanisms at interfaces
- Utilize microstructure control to impart radiation resistance to structural materials for ANES
- Innovative experimental methods for dynamic, *in situ* measurements of fundamental properties

- Predict microstructural and chemical evolution in actinide fuel, cladding and structural materials during irradiation
- Identify self-protective interfacial reaction mechanisms capable of providing universal stability in extreme environments
- Improve understanding of coordination geometry, covalency, oxidation state, and cooperative effects of actinides to devise next generation separation methods.
- Predict the behavior of waste forms over millennia

Applied Research / Technology Maturation & Deployment

- Rational design and development of reactor fuels
- Verified and validated modules for reactor-level multi-scale simulations
- Develop 3D fuel performance code
- Laboratory-scale sample fabrication and characterization with relevant post-irradiation examination of samples
- Demonstrate new separation systems at bench scale
- Demonstrate at-scale waste-form performance in deep geologic laboratory

- Demonstrate the scaling to production-scale by process prototyping
- Develop and validate fuel licensing code for design and safety basis
- Fabricate and characterize lead test assemblies (LTAs)
- Irradiate lead test assemblies in prototypic environment
- Couple waste-form performance to design and performance of a repository.

Office of Science
BES

Technology Offices
NE

Materials Under Extreme Environments

Discovery Research

- Dynamics of excitation and relaxation under extreme flux
- Fundamental limits of dielectric performance
- Bond-energy-charge relationships over relevant conditions
- Complex chemistry and physics of degradation
- Multi-dimensional in-situ characterization tools
- Extreme environments as probes of materials behavior
- Self assembled multi-paradigm algorithms for understanding materials performance
- Atomic level understanding of dynamic behavior
- Fundamental knowledge of non-equilibrium systems
- Novel states of matter in extreme magnetic fields
- Design and synthesis of transformational materials

Use-inspired Basic Research

- Achieving stable, non-reacting surfaces
- Exploit kinetically states far from equilibrium
- Mitigating materials degradation under extreme conditions
- Simulating and measuring dynamics at the same length and time scales
- Understanding dynamic behavior across interfaces
- Enabling a new generation of non-traditional materials for extreme environments
- Development of highly robust materials for extreme environments
- Harnessing extreme conditions to create new materials with revolutionary functionality

Applied Research

- Application of models and computational tools for system design and diagnostics for energy technologies requiring high strength and temperature
- Material evaluation and process development for radiation resistant materials for use in solar thermal, defense, nuclear reactors, and waste storage
- Improve long-term stability under extreme temperature, cyclic loads, pressure, chemical reactivity and electromagnetic field for energy generation and use
- Develop and apply novel materials processes and manufacturing technologies
- Proof of technology concepts with improved performance and reduced cost for use in extreme conditions

Technology Maturation & Deployment

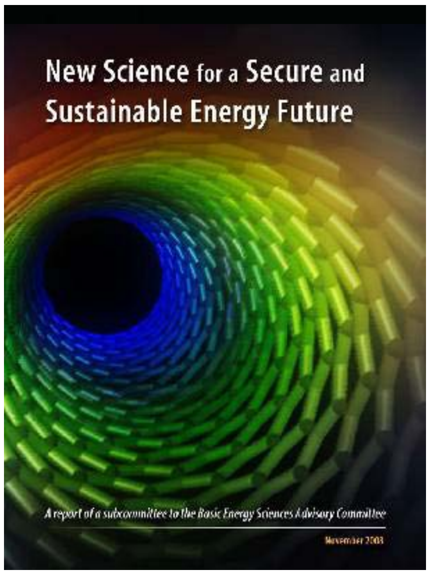
- Demonstrate energy production and utilization systems operating at high efficiency
- Support the establishment of domestic manufacturing capabilities for highly robust components and systems
- Development and deployment of reliable, high-capacity distribution and storage systems for centralized and distributed power sources
- Develop long-life, low-cost reliable, environmentally friendly recyclable processes for energy applications
- Computer validation of multifunctional materials performance for applications in extreme environments

Geosciences

Discovery Research	Use-inspired Basic Research	Applied Research	Technology Maturation & Deployment
Microscopic basis of macroscopic complexity - scaling	Mineral-fluid interface complexity and dynamics	Develop and test methods for assessing storage capacity and for monitoring containment of CO_2 storage	Develop site selection criteria
Highly reactive subsurface materials and environments	Nanoparticulate and colloid chemistry and physics	Develop remediation methods to ensure permanent storage	Develop storage and operating engineering approaches
Thermodynamics of the solute-to-solid continuum	Dynamic imaging of flow and transport	Demonstrate procedures for characterizing storage reservoirs and seals	Storage demonstrations
Computational geochemistry of complex moving fluids within porous solids	Transport properties and *in situ* characterization of fluid trapping, isolation and immobilization	Integrated models for waste performance prediction and confirmation	Apply assessment protocols and technologies for the lifecycle of projects
Integrated analysis, modeling and monitoring of geologic systems	Fluid-induced rock deformation	Radionuclide partitioning in repository environments.	Evaluate release of radionuclide inventory from the repository
Simulation of multi-scale systems for ultra-long times	Biogeochemical in extreme subsurface environments	Waste form stability and release models.	Assess corrosion/ alteration of engineered materials
		Incorporate new conceptual models into uncertainty assessments.	Long-term safety/risk assessment for emplacement of energy system by-products.

Office of Science — FE, RW, EM, EERE

Additional Workshops and Resources



New Science for a Secure and Sustainable Energy Future

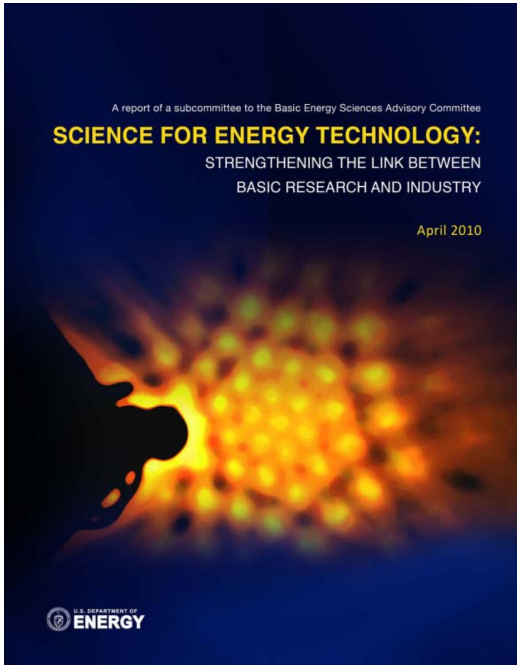
Goals:

- 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

Science for Energy Technology – BESAC Report - April 2010



Science for Energy Technology:
Strengthening the Link between Basic Research and Industry

Overarching Themes:

- Research to develop foundational scientific understanding of at-scale production challenges in existing materials and processes for emergent energy technologies
- Research that extends beyond empiricism towards the fundamental understanding of lifetime prediction of materials in extreme environments, especially aging, degradation, and failure
- Research aimed at the discovery of specific new materials or chemical processes with targeted functionality that would lower the cost and improve the efficiency of clean energy technologies

Proposed Research Directions: Advanced Nuclear Energy (Kurt Edsinger, EPRI)

- Materials Degradation Mechanisms
- Advanced Irradiation Effects Scaling
- Back End of the Fuel Cycle

DOE's Energy Priorities and Goals

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: 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
  - 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

Basic Sciences Underpinning Technology

- **Coordination between basic science and applied research and technology is an important mechanism by which to translate transformational discoveries into practical devices**

- **Many activities facilitate cooperation and coordination between BES and the technology programs**
  - Joint efforts in strategic planning (e.g., Basic Research Needs workshops)
  - Solicitation development
  - Reciprocal staff participation in proposal review activities
  - Joint program contractors meetings
  - Joint SBIR topics
  - Participation by BES researchers in merit reviews and meetings

- **Co-funding and co-siting of research by BES and DOE technology programs at DOE labs or universities, has proven to be a viable approach to facilitate close integration of basic and applied research through sharing of resources, expertise, and knowledge of research breakthroughs and program needs.**

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

Radiation Effects Research at BES

- **Funding for Radiation Effects in Materials includes 4 Energy Frontier Research Centers**
  - Stocks (ORNL)
  - Allen, interim (INL)
  - Nastasi (LANL)
  - Burns (Notre Dame)
- **Complement to NE research objectives**
  - BES: Understand radiation resistance in materials
  - NE: Design radiation resistant material
- **Variety of Core Projects Ranging from studying the Fundamentals of Radiation Damage in Alloys/Ceramics to Stress Corrosion Cracking**
  - 6 University Grants and 7 Laboratory FWPs
- **Mechanical Behavior and Radiation Effects Program Contractors' Meeting to be held Sept. 28-Oct. 1, 2010**

Four Energy Frontier Research Centers – Advanced Nuclear Energy Systems

Todd Allen (interim), Idaho National Lab

Center for Materials Science of Nuclear Fuel

Peter Burns, Univ. of Notre Dame

Materials Science of Actinides (MSA)

Malcolm Stocks, ORNL

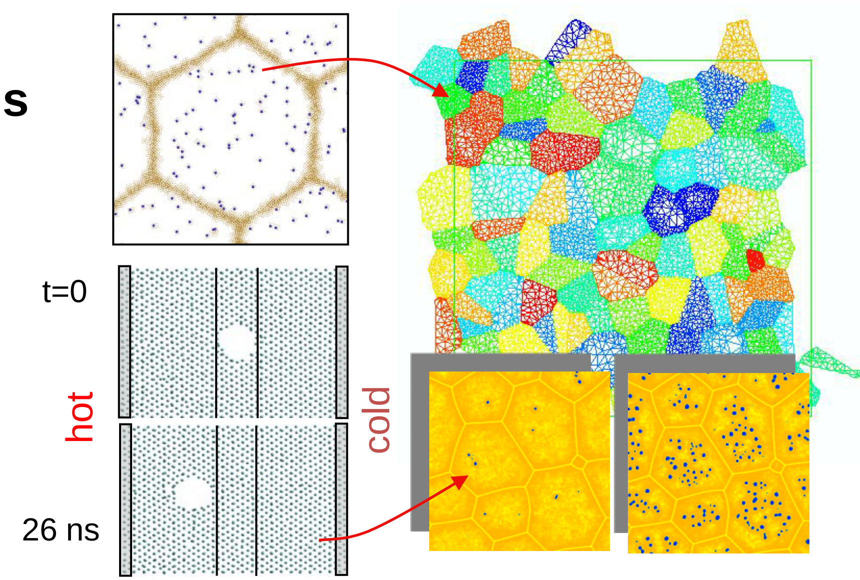
Center for Defect Physics in Structural Materials (CDP)

Michael Nastasi, LANL

Center for Materials at Irradiation and Mechanical Extremes (MIME)

Center for Materials Science of Nuclear Fuel
Todd Allen (Idaho National Laboratory)

Summary: **The central theme of the Center is *'Microstructure Science under Irradiation'*, i.e., the determination of how concurrent microstructure formation and evolution under irradiation control the thermo-mechanical behavior of UO_2 as a model nuclear-fuel material.**



RESEARCH PLAN AND DIRECTIONS

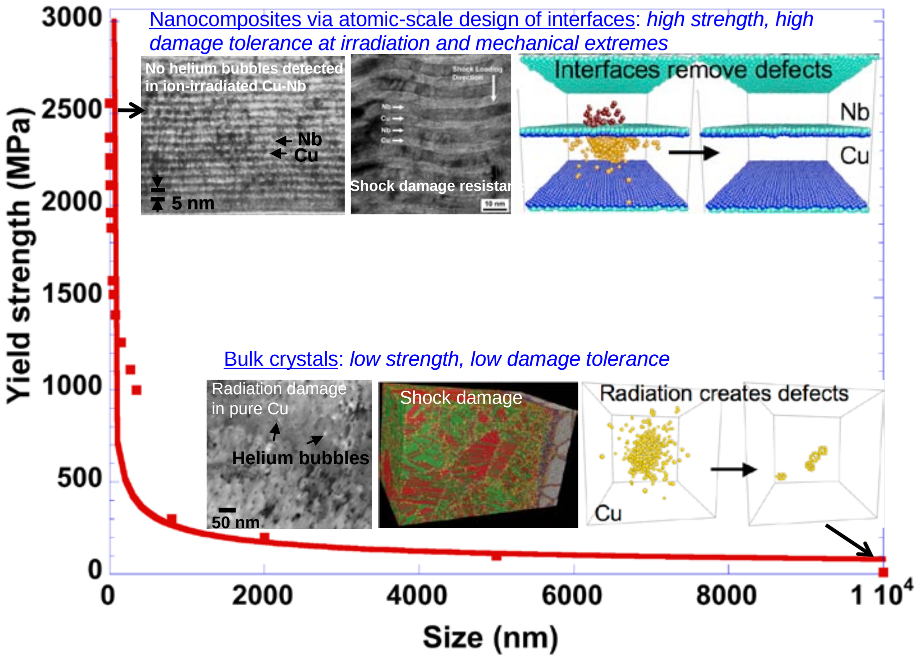
Develop an *experimentally validated, multi-scale modeling approach* for micro-structure evolution under irradiation (void-, fission-gas and phase behavior, stress development, ...) and predict how these affect, e.g., thermal transport. Incorporation of microstructural processes based on atomic-level mechanisms is critical towards developing a *predictive* fuels-performance capability.

U.S. DEPARTMENT OF ENERGY | Office of Science

Materials at Irradiation and Mechanical Extremes
Michael Nastasi (LANL)

***Summary statement*:**

The purpose of this EFRC is to understand, at the atomic scale, the behavior of materials subjected to extreme radiation doses and mechanical stress in order to synthesize new materials that can tolerate such conditions.



The EFRC will develop a fundamental understanding of how atomic structure and energetics of interfaces contribute to defect and damage evolution in materials, and use this information to design nanostructured materials with tailored response at irradiation and mechanical extremes with potential applications in next generation of nuclear power reactors, transportation, energy and defense.

Materials Science of Actinides
Peter C. Burns (University of Notre Dame)

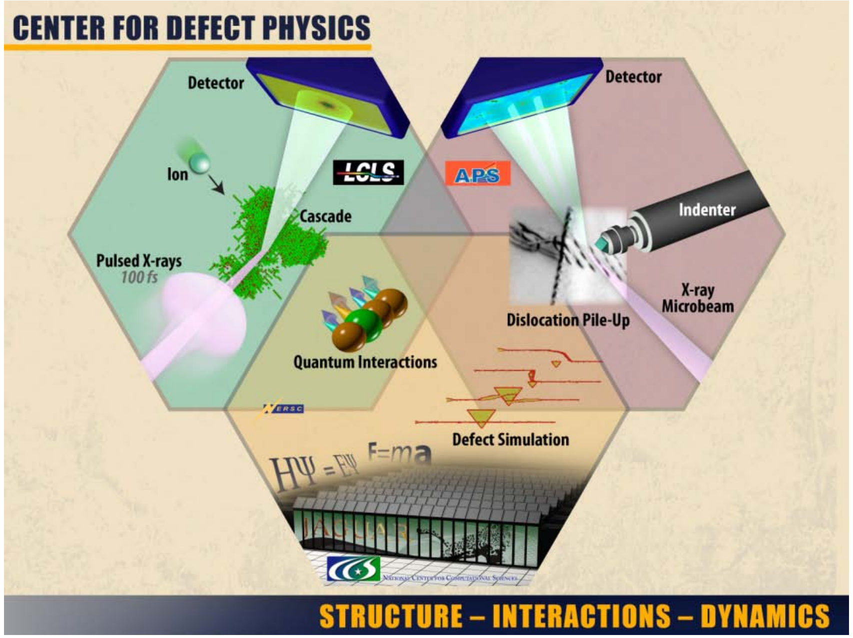
The Materials Science of Actinides EFRC seeks to understand and control, at the nanoscale, materials that contain actinides (radioactive heavy elements such as uranium and plutonium) to lay the scientific foundation for advanced nuclear energy systems.

RESEARCH PLAN AND DIRECTIONS

This EFRC blends experimental and computational approaches to study highly complex actinide materials (such as materials for fuels, waste forms, or separations), with an emphasis on the nanoscale. The behavior and properties of such materials in extreme environments of radiation and pressure is a major focus of this research.

Center for Defect Physics
G. Malcolm Stocks (ORNL)

Our goal is to provide a fundamental understanding of materials' defects, defect interactions, and defect dynamics, thereby enabling atomistic control and manipulation of defects and the charting of new pathways to the development of improved materials – materials with ultra-high strength, toughness, and radiation resistance.



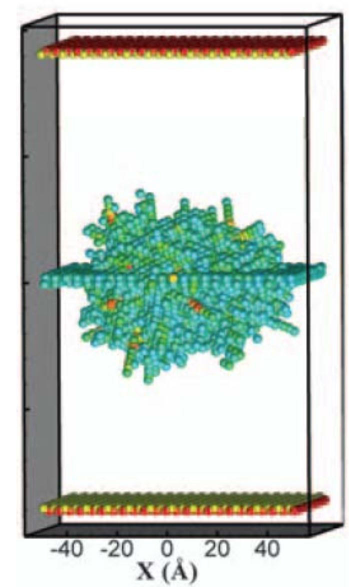
We deploy first-of-their-kind measurements and *ab initio* quantum calculations of the structure, interactions, and dynamics of defects in structural materials. The Center focuses on three interrelated thrust areas:

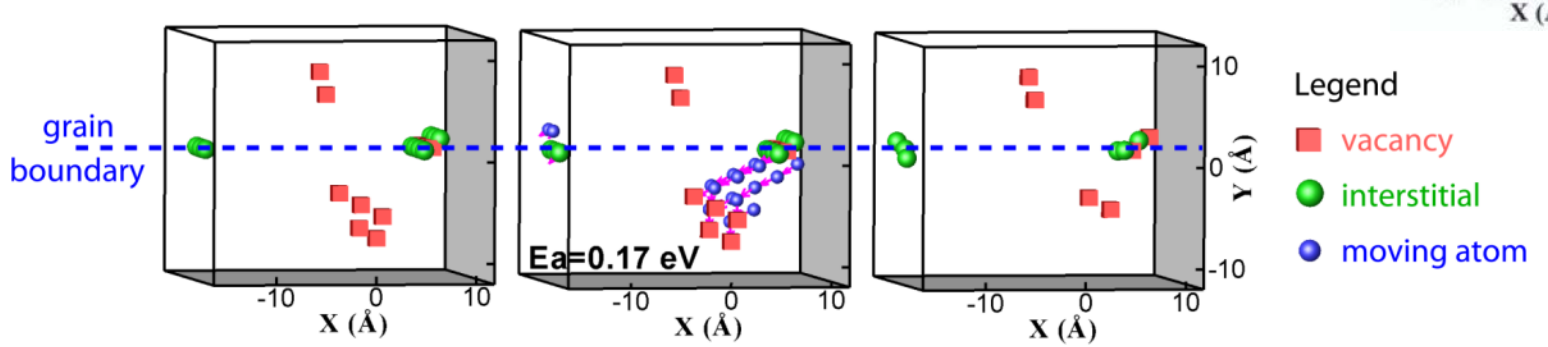
- *Fundamental Physics of Defect Formation and Evolution during Irradiation*
- *Fundamental Physics of Defect Interactions during Deformation*
- *Quantum Theory of Defects and their Interactions*

Understanding Radiation Resistance in Materials

Energy Frontier Research Center for Materials at Irradiation and Mechanical Extremes

- Key to radiation resistance is efficient recombination of vacancies and interstitials (point defects) created by damage cascades formed when neutrons collide with atoms in materials . In this early EFRC result, grain boundaries were found to enable a surprising mechanism for increasing point-defect recombination and potentially imparting greater radiation resistance to materials
- After a simulated collision cascade (at right, showing displaced atoms 0.5 ps after the cascade initiation), fast-moving interstitials move quickly to a nearby boundary (below, at left). Slower-moving vacancies remain in the bulk material.
- This research showed that a grain boundary loaded with interstitials emits these interstitials (below, center) via a newly-discovered low-energy mechanism to annihilate nearby vacancies much faster than other mechanisms (below, at right)
- This new mechanism may explain the enhanced radiation resistance observed in nanocrystalline materials with large numbers of grain boundaries



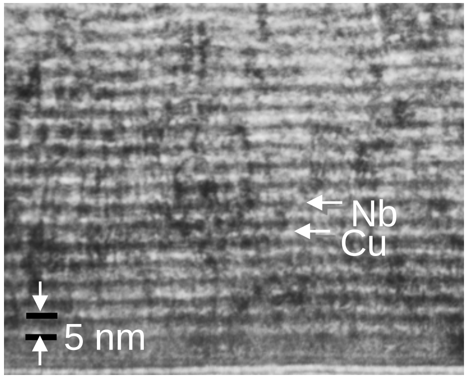


Bai, X.M., Voter, A.F., Hoagland, R.G., Nastasi, M. and Uberuaga, B.P., “Efficient Annealing of Radiation Damage Near Grain Boundaries via Interstitial Emission”, *Science*, available online 3/25/2010

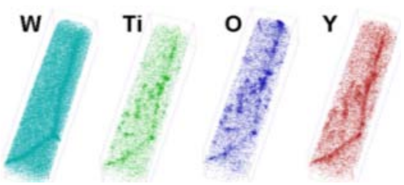
Nastasi (LANL)

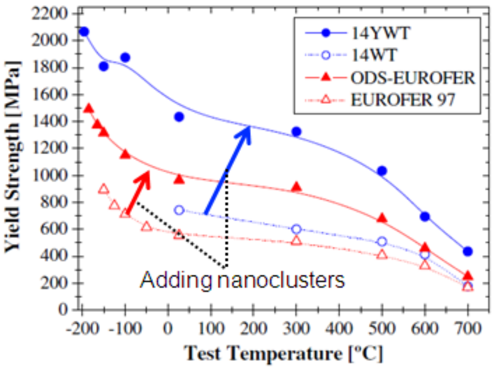
Nanostructured Materials for Strength and Radiation Resistance in Metals

5 nm multilayer structures of Cu-Nb exhibit high strength and resistance to radiation damage



En-Gang Fu et al., *Mat. Sci and Eng. A*, 493, 283 (2008)





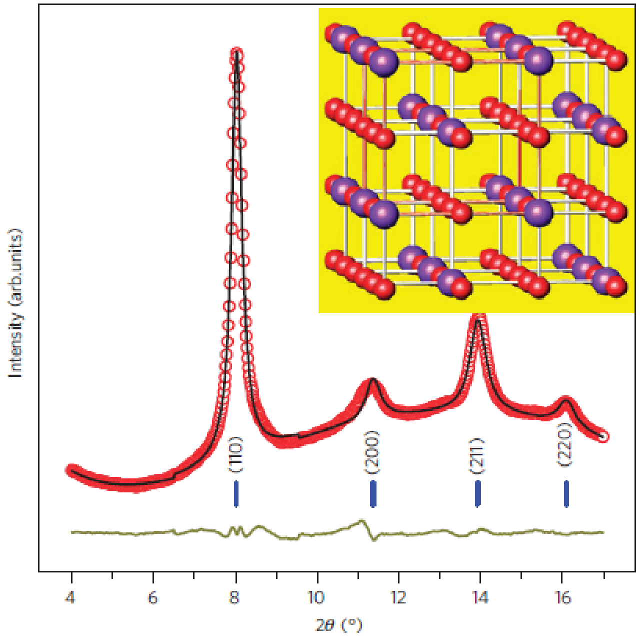
Stable nanoclusters (~2-4 nm in size) are found in ferritic alloys prepared by mechanical alloying and serve to increase strength even after long times at high temperatures

Xu et al, *Phys Rev. B*, 79 (2) 020204 (2009)

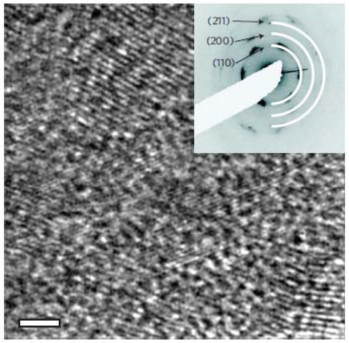
- **Materials with nano-scale features such as multi-layers (e.g. Cu-Nb) or oxide-based nanoclusters have been found to posses remarkable strength, even at high temperatures, and resist changes due to radiation far better than their conventional counterparts.**

- **Research is ongoing to better understand how interfaces can lead to these improvements, which may result in structural materials that retain their properties in the extreme environments found in advanced nuclear energy systems.**

Ambient Condition Stabilization of High-Pressure Phase in $Gd_2Zr_20_7$ by Utilization of Extreme Environments



(above) XRD data (red circles) and model (black line(for cubic x-phase (crystal structure model) stabilized at room temperature. (right) TEM image and corresponding diffraction pattern (confirming nanocrystalline structure) of recovered sample.



•High-pressure and high-temperature phases show unusual physical and chemical properties, but they are often difficult to 'quench' to ambient conditions.

•A new approach was used to stabilize a high-pressure phase , bombarding the $Gd_2Zr_20_7$ with very high-energy heavy ions (e.g. 20 GeV Xe ions) while the material was held at pressures up to 40 GPa.

•The previously unquenchable cubic high-pressure phase was recovered after release of pressure as revealed by XRD (top left) and TEM (below left), which also indicated that the combination of pressure and irradiation created a nanocrystalline structure.

•Quantum-mechanical calculations confirm that the surface energy at the nanoscale is the cause of the remarkable stabilization of the high-pressure phase. The combined use of high pressure and high-energy ion irradiation provides a new means for manipulating and stabilizing new materials to ambient conditions that otherwise could not be recovered.

Rod Ewing's Group (UMich)

M. Laing et al., "*Nanoscale manipulation of the properties of solids at high pressure with relativistic heavy ions*", **Nature Materials**, Vol 8, (2009) p. 793

Office of Science FY 2011 Investment Highlights

The FY 2011 budget advances discovery science and invests in science for national needs in energy, climate, and the environment; national scientific user facilities; and education and workforce development.

Discovery science addressing national priorities

- Energy Innovation Hub for Batteries and Energy Storage (+$34,020K, BES)
- Enhanced activities in climate science and modeling (Regional and Global Climate Modeling, +$6,495K; Earth System Modeling, +$9,015K; Atmospheric System Research, +$1,944K; ARM Climate Research Facility, +$3,961K; BER)
- Individual investigator, small group, and Energy Frontier Research Centers (EFRCs) in areas complementing the initial suite of 46 EFRCs awarded in FY 2009 (+$66,246K, BES)
- Leadership Computing Facilities operations and preparation for next generation of computer acquisitions for S&T modeling and simulation ($34,832K, ASCR)
- Multiscale modeling of combustion and advanced engine systems (+$20,000K, BES)

Scientific user facilities—21st century tools of science, technology, and engineering

- Facility construction is fully funded; projects are meeting baselines
- 28 scientific user facilities will serve more than 26,000 users
- Several new projects and Major Items of Equipment are initiated (e.g., the Long Baseline Neutrino Experiment, +$12,000K, HEP)

Education and workforce development

- Expansions of the SC Graduate Fellowship Program (+$10,000K, 170 new awards, WDTS) and the SC Early Career Research Program (+$16,000K, 60 new awards, funded in all of the SC research programs)

New BES Research Investments Address Critical Needs

An FY 2011 BES call will cover a broad range of research awards including new EFRCs

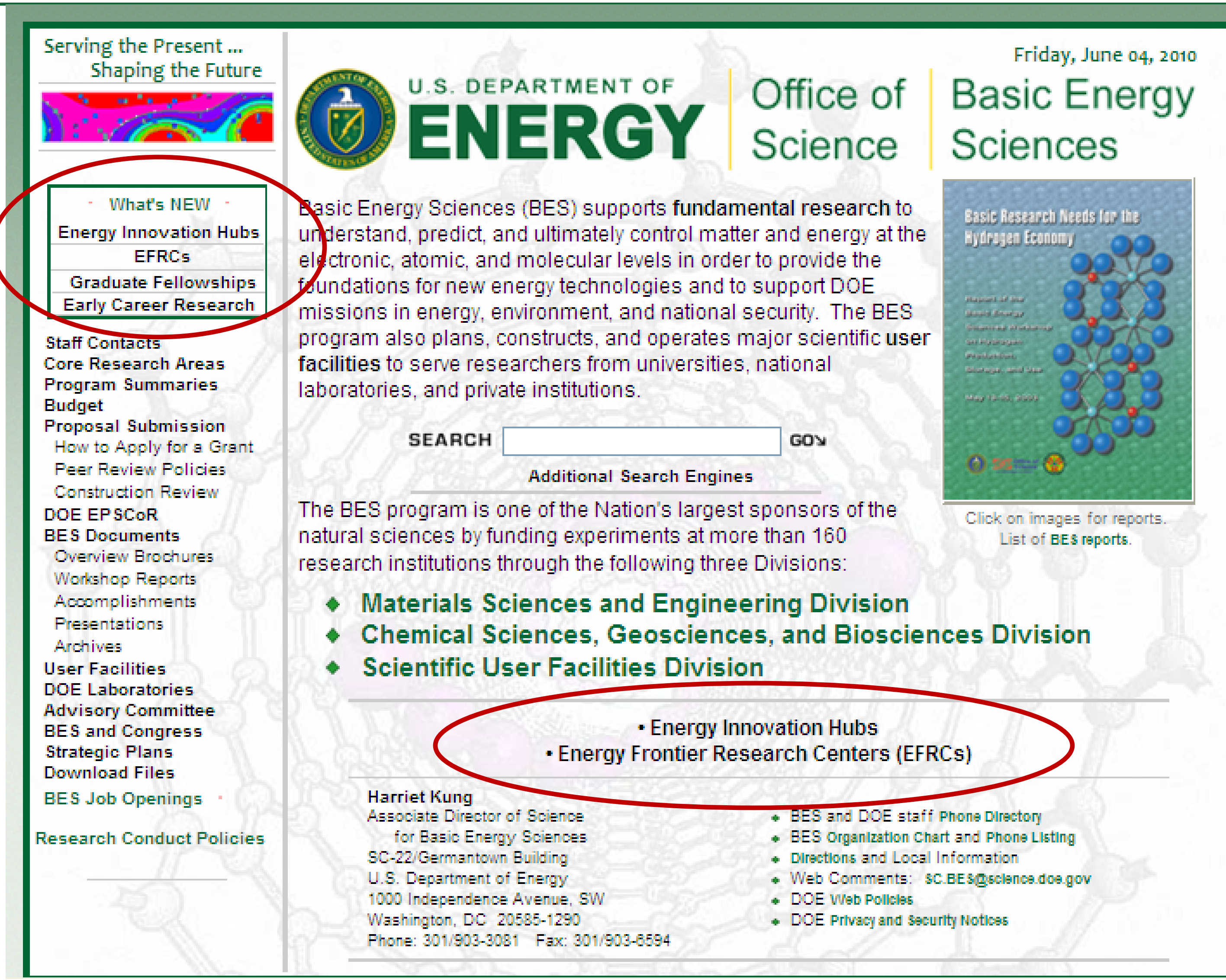
About $66 million will be competed in the BES Program to support single investigators, small groups, and additional Energy Frontier Research Centers in the following areas:

1. **Discovery and development of new materials**
   The FY 2011 solicitation will emphasize new synthesis capabilities, including bio-inspired approaches, for science-driven materials discovery and synthesis. Research will include crystalline materials, which have broad technology applications and enable the exploration of novel states of matter.

2. **Research for energy applications**
   The FY 2011 solicitation will emphasize fundamental science related to:
   - **Carbon capture**, including the rational design of novel materials and separation processes for post-combustion CO_2 capture in existing power plants and catalysis and separation research for novel carbon capture schemes to aid the design of future power plants.
   - **Advanced nuclear energy systems** including radiation resistant materials in fission and fusion applications and separation science and heavy element chemistry for fuel cycles.

Awards will be competitively solicited via Funding Opportunity Announcements following the FY 2011 appropriation

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



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* Or just Google "DOE + BES"