The Role of Advanced Computing in Basic Energy Sciences

March 31, 2010

Harriet Kung
Director, Basic Energy Sciences
Office of Science, U.S. DOE

Basic Energy Sciences Mission

The mission of the Basic Energy Sciences program is 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:

- To discover and design new materials and molecular assemblies with novel structures, functions, and properties.
- To conceptualize, calculate, and predict processes underlying physical and chemical transformations.
- To 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 conceive, plan, design, construct, and operate scientific user facilities to probe the most fundamental electronic and atomic properties of materials at extreme limits of time, space, and energy resolution through x-ray, neutron, and electron beam scattering.
- To foster integration of the basic research conducted in the program with research in NNSA and the DOE technology programs.

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; △ 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; 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 & 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 & 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

Photo- and Bio-Chemistry

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**: Lester Morss; ● Norm Edelstein, LBNL
- **Separations and Analysis**: Bill Millman; △ Larry Rahn, SNL
- **Geosciences**: Nick Woodward; ● Jennifer Blank, LBNL
- **Technology Office Coordination**: Marvin Singer; Vacant

LEGEND

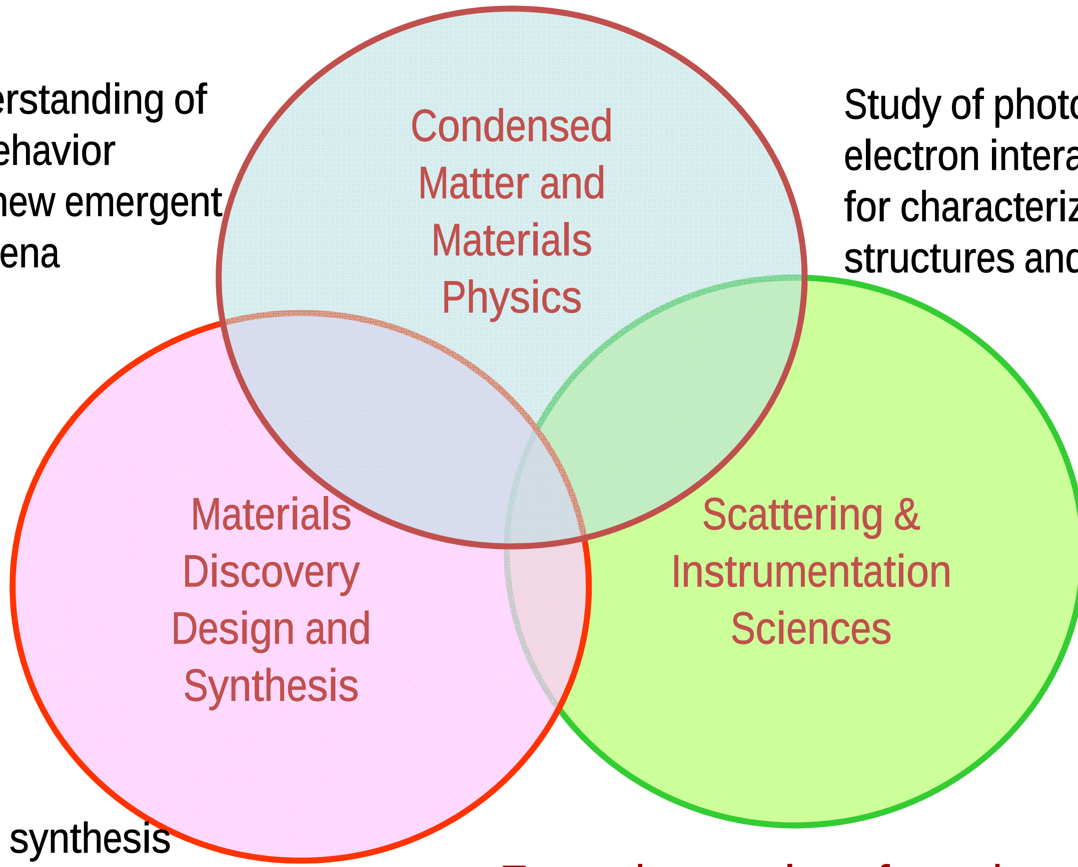
- ◆ Detailee (from DOE laboratories)
- ■ Detailee, ½ time, not at HQ
- ● Detailee, ¼ time, not at HQ
- ◆ On detail to EERE/SETP, 30%
- △ IPA (Interagency Personnel Act)
- ☆ On active military duty
- P.A. Program Assistant

March 2010

Materials Sciences and Engineering

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

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

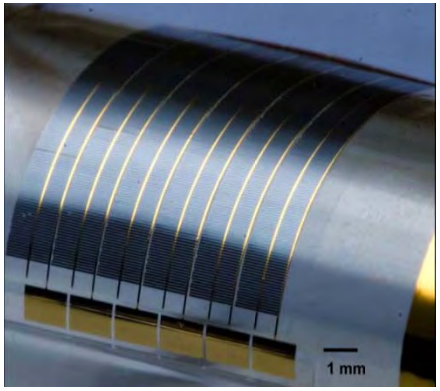


Rational design and synthesis of new materials via physical, chemical, and biomolecular routes

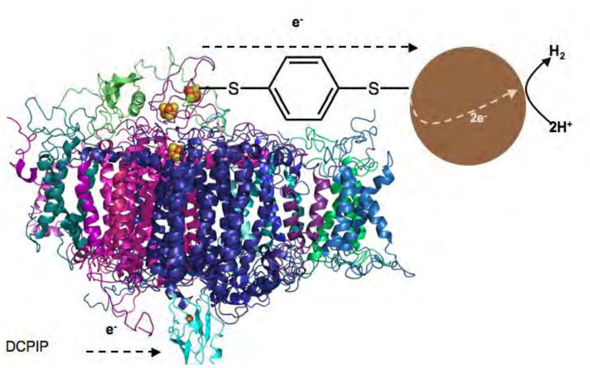
Teams have unique focus but some common, synergistic scientific themes:

- Correlation phenomena

Key Areas of Research in Materials Discovery, Design, and Synthesis

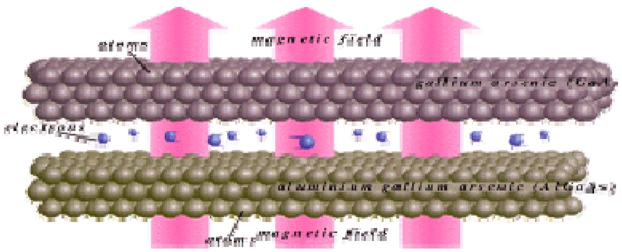


- Develop scientific strategies to fabricate macroscopic materials with nanometer scale precision
- Establish fundamental understanding of thermodynamics, kinetics and dynamics of self-assembly
- Understand fundamental principles to produce materials with precisely controlled defects
- Develop multi-component, multi-functional materials
- Develop new classes of materials and innovative architectures that can revolutionize energy conversion, storage and transfer

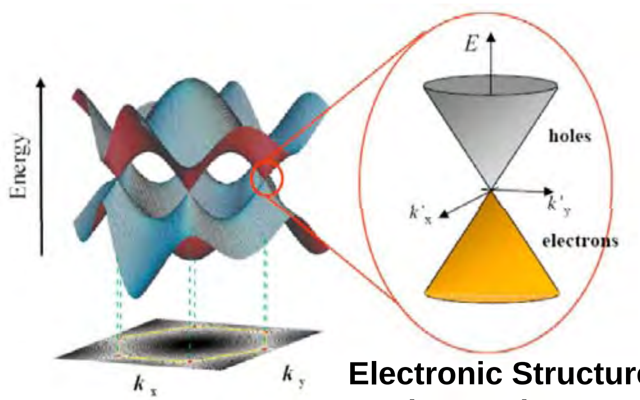


PS-I covalently attached to nanoparticle catalysts via a molecular wire yields 75% of plant electron transfer rates resulting in photo-generated hydrogen at ~1700 X current

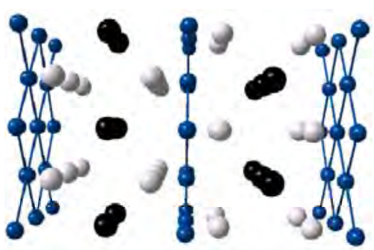
Key Areas of Research in Condensed Matter and Materials Physics



Two-Dimensional Electrons in Gallium Arsenide Semiconductors



Electronic Structure in Graphene

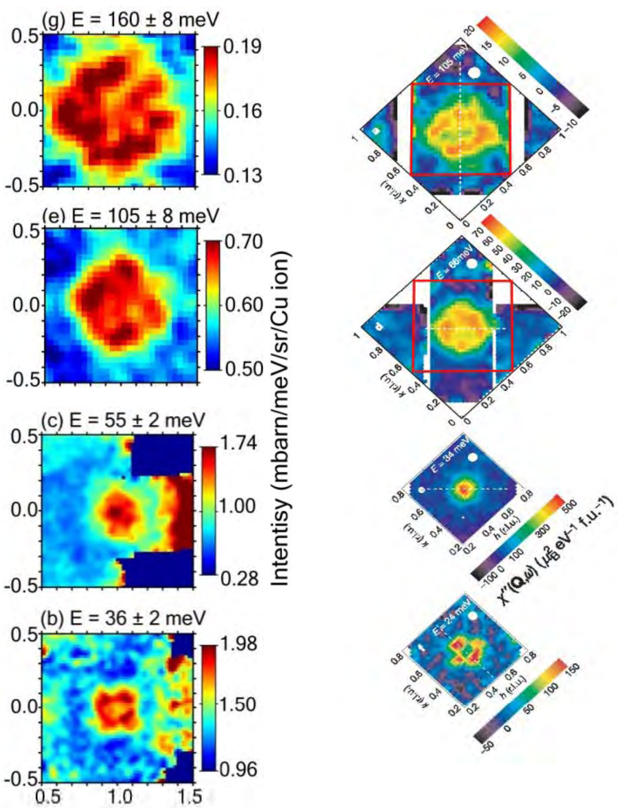


Tetragonal structure with square nets of $Fe^{2+\,I}$ in $BaFe_{1.84}Co_{0.16}As_2$

- Develop a detailed understanding of the phenomena of superconductivity and magnetism
- Understand the influence of defects on materials at the atomic scale
- Investigate the properties of materials under extreme environments
- Understand and control the structure and properties of materials at the nanoscale
- Design, fabrication and characterization of metamaterials

Key Areas of Research in Scattering and Instrumentation Sciences

Magnetic Fluctuations in Superconductors



LBCO **YBCO**

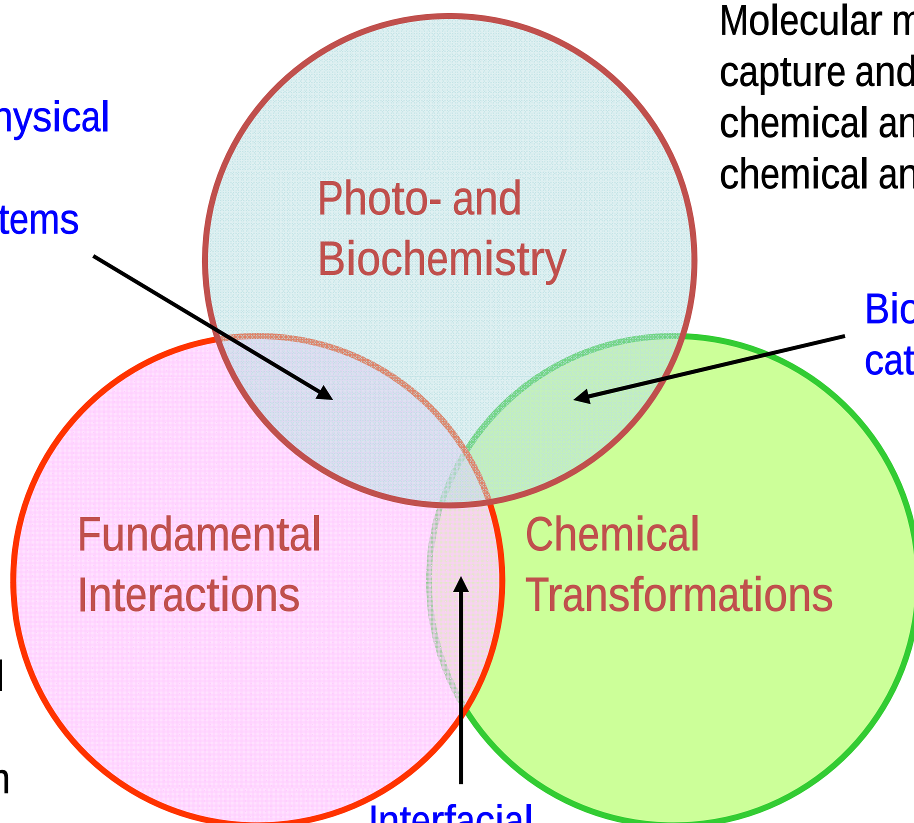
Neutron scattering studies demonstrate universal magnetic excitation spectrum

- Utilize scanning probes to elucidate mechanisms that control phenomena in correlated electron systems
- Develop a structural and dynamical understanding of nanostructured materials
- Understand dynamics and materials functionality using ultrafast diffraction, spectroscopy and imaging techniques
- Unify the complementary information obtained through multiple techniques

Chemical Sciences, Geosciences and Biosciences

Application of physical science tools to biochemical systems

Molecular mechanisms of light capture and its conversion to chemical and electrical energy via chemical and biochemical pathways



Biomimetic catalytic systems

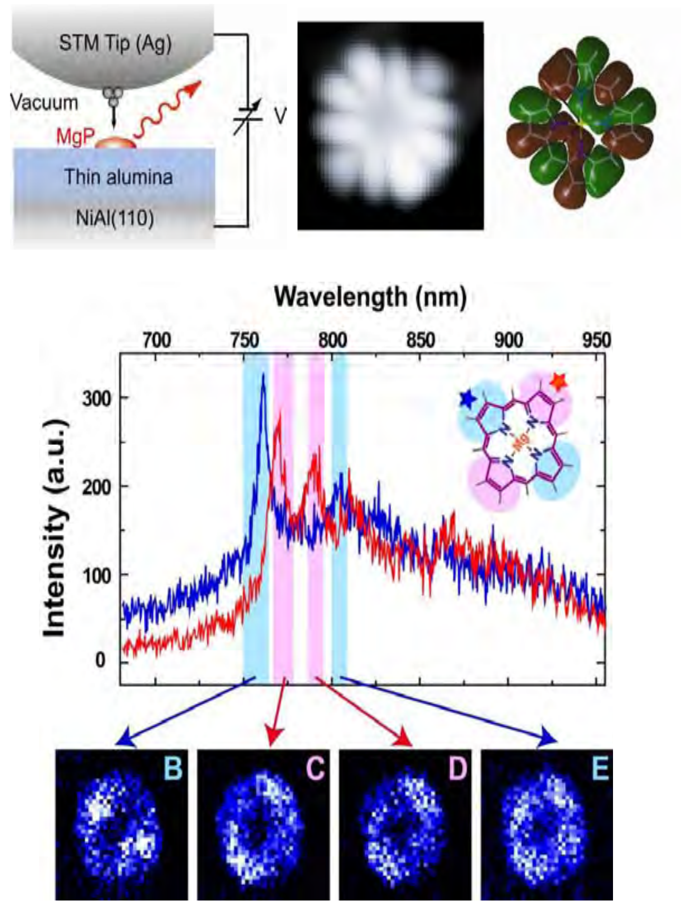
Structural and dynamical studies of atoms, molecules, and nanostructures; description of their interactions with external stimuli (photons, electrons) at full quantum detail

Characterization, control, and optimization of chemical transformations, from catalysis to geochemistry

Interfacial nanoscale chemistry

Division-wide themes: chemical imaging; ultrafast chemical sciences; nanoscale science; catalytic science; theory, modeling, & simulation; synthesis

Key Areas of Research in Fundamental Interactions



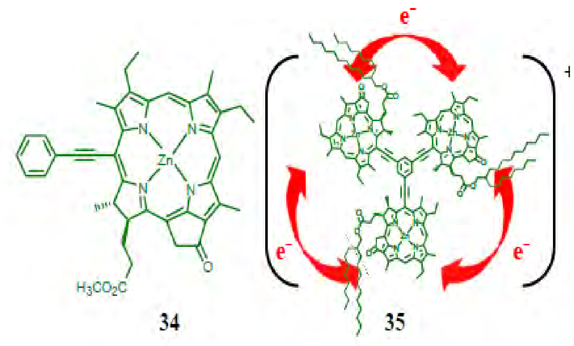
Scanning tunneling microscope images produced while monitoring the emission spectrum of a single molecule show, with atomic resolution, different spectra emitted from different locations on the molecule, giving an unprecedented atomic-level view of the coupling of electronic and vibrational motion. (Wilson Ho, UC Irvine)

models and computational tools to predict rates, products, and dynamics of chemical processes in the gas phase.

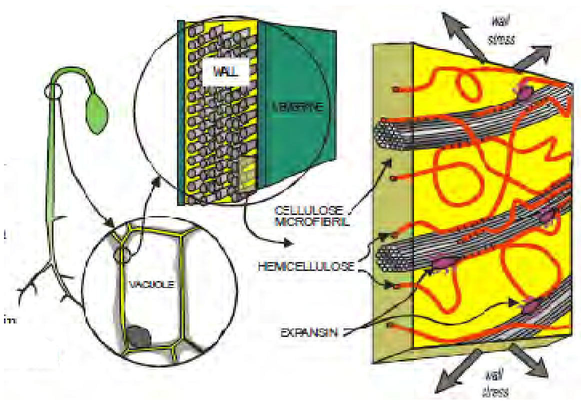
- Develop a molecular-level understanding

- Theory and computational methods to advance research goals across the Division.

Key Areas of Research in Photo- and Bio-Chemistry



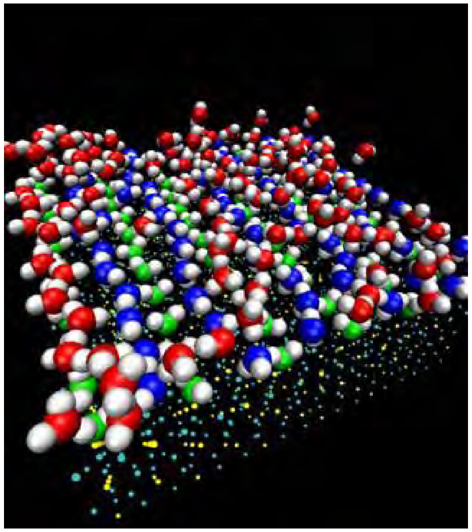
Chlorophyll monomer and trimer building block for supramolecular charge transport systems. (Tiede et al, ANL)



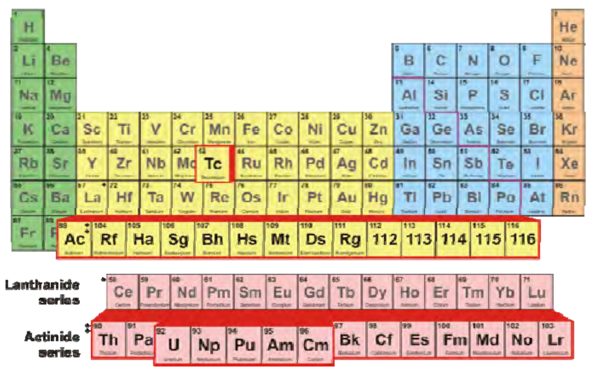
Mechanism of plant cell wall loosening by the protein expansin, which modulates non-covalent linkages between hemi-cellulose and celluose (Cosgrove, Penn State).

- Basic research in solar photochemistry with the goal of creating viable and efficient artificial photosynthetic systems

Key Areas of Research in Chemical Transformations



Molecular dynamics simulation of water on a mineral surface based on neutron scattering data from the SNS



Actinide elements of interest to advanced fuel cycle

- Resolving the f-electron challenge to understand the chemistry and physics of actinide compounds

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BES Research — Science for Discovery & National Needs

Three Major Types of Research Thrusts

increasing progression of scientific scope and level of effort

- **Core Research**

  Support single investigator and small group projects to pursue their specific research interests.

  - Enable seminal advances in the core disciplines of the basic energy sciences—materials sciences and engineering, chemistry, and aspects of geosciences and biosciences. Accelerator and detector R&D is also supported.
  - Build research programs that provide world-class, peer-reviewed research results cognizant of both DOE mission needs and new scientific opportunities. Scientific discoveries at the frontiers of these disciplines establish the knowledge foundation to spur future innovations and inventions.

- **Energy Frontier Research Centers**

  $2-5 million-per-year research centers, established in 2009, focused on fundamental research related to energy

  - Multi-investigator and multi-disciplinary centers to harness the most basic and advanced discovery research in a concerted effort to accelerate the scientific breakthroughs needed to create advanced energy technologies. Bring together critical masses of researchers to conduct fundamental energy research in a new era of grand challenge science and use-inspired energy research.
  - EFRCs are overseen by program staff, who are managed centrally within BES to ensure a unified management strategy and structure.

- **Energy Innovation Hubs**

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

  - Hubs comprise a larger set of investigators spanning science, engineering, and other disciplines focused on a single critical national need identified by the Department; each Hub is expected to become a world leading R&D center in its topical area to develop a complete energy system.
  - With robust links to industry, the highly integrated Hubs can bridge the gap between basic scientific breakthroughs and industrial commercialization.

BES Scientific User Facilities

<u>Light sources</u>
Stanford Synchrotron Radiation Laboratory (SLAC)
National Synchrotron Light Source (BNL)
National Synchrotron Light Source II (BNL)
(start construction FY 2010)
Advanced Light Source (LBNL)
Advanced Photon Source (ANL)
Linac Coherent Light Source (SLAC)

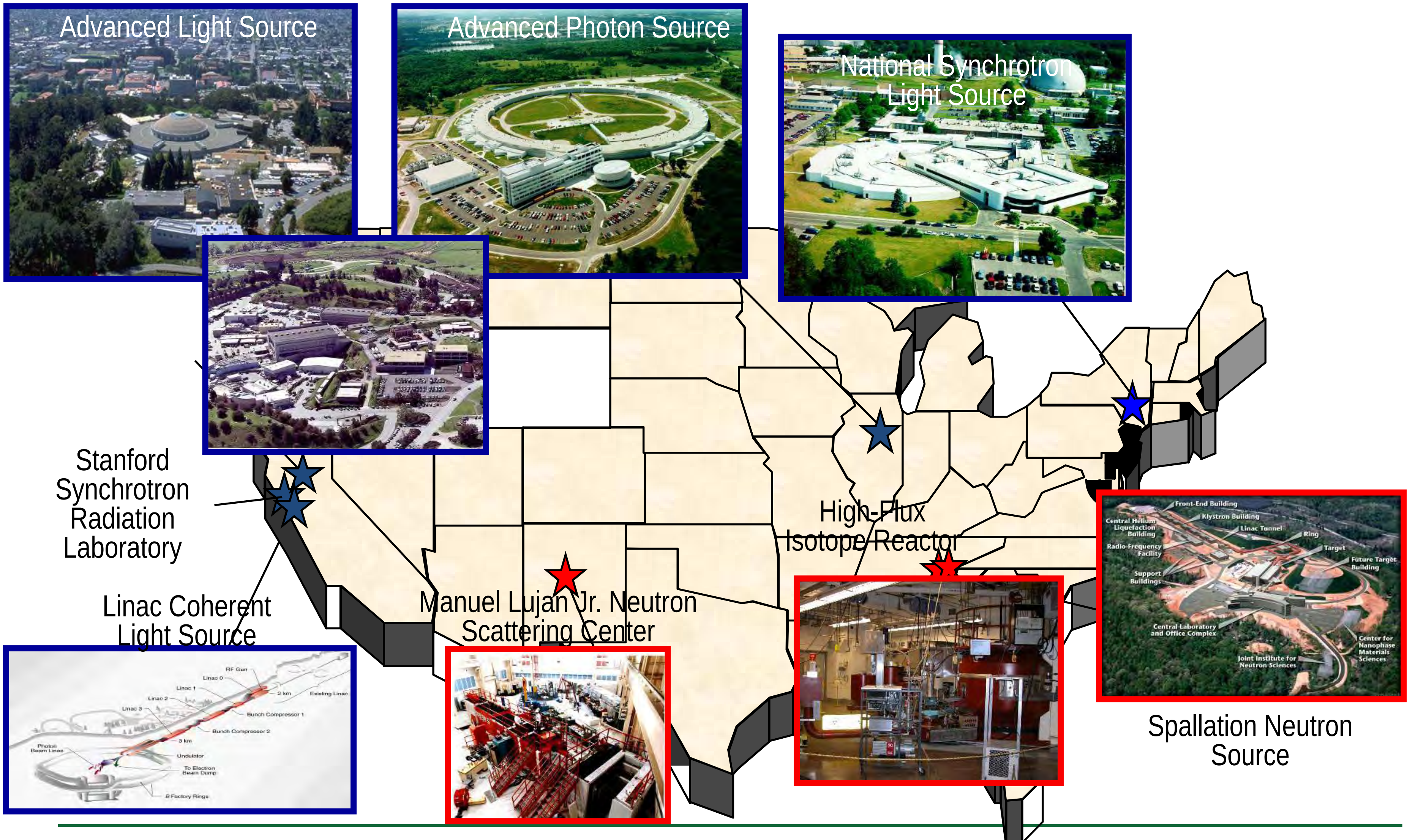
<u>Neutron sources</u>
Manuel Lujan, Jr. Neutron Scattering Center (LANL)
High Flux Isotope Reactor (ORNL)
Spallation Neutron Source (ORNL)

<u>Electron beam sources</u>
Electron Microscopy Center for Materials Research (ANL)
National Center for Electron Microscopy (LBNL)
Shared Research Equipment Program (ORNL)

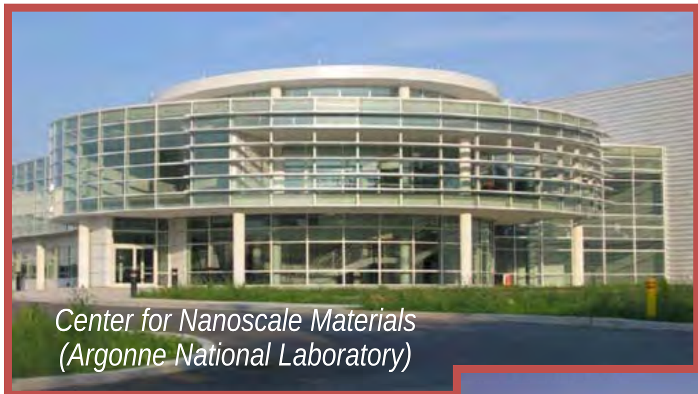
<u>Nanoscale Science Research Centers</u>
Center for Nanophase Materials Sciences (ORNL)
Molecular Foundry (LBNL)
Center for Integrated Nanotechnologies (SNL/A & LANL)
Center for Functional Nanomaterials (BNL)
Center for Nanoscale Materials (ANL)

Artist's drawings of National Synchrotron Light Source-II (top) and Linac Coherent Light Source (bottom)

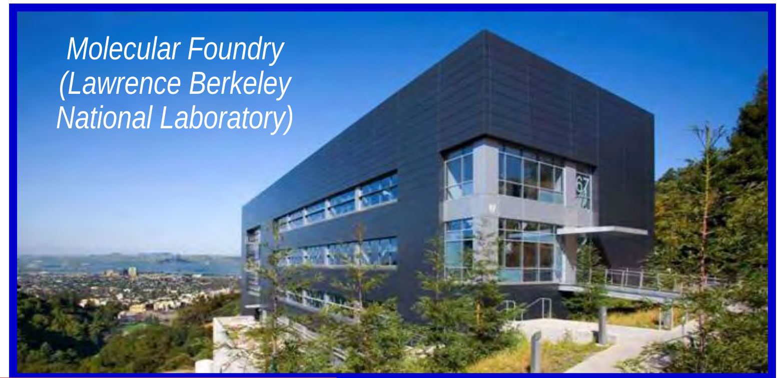
BES Facilities for X-ray and Neutron Scattering



Nanoscale Science Research Centers



Center for Nanoscale Materials (Argonne National Laboratory)



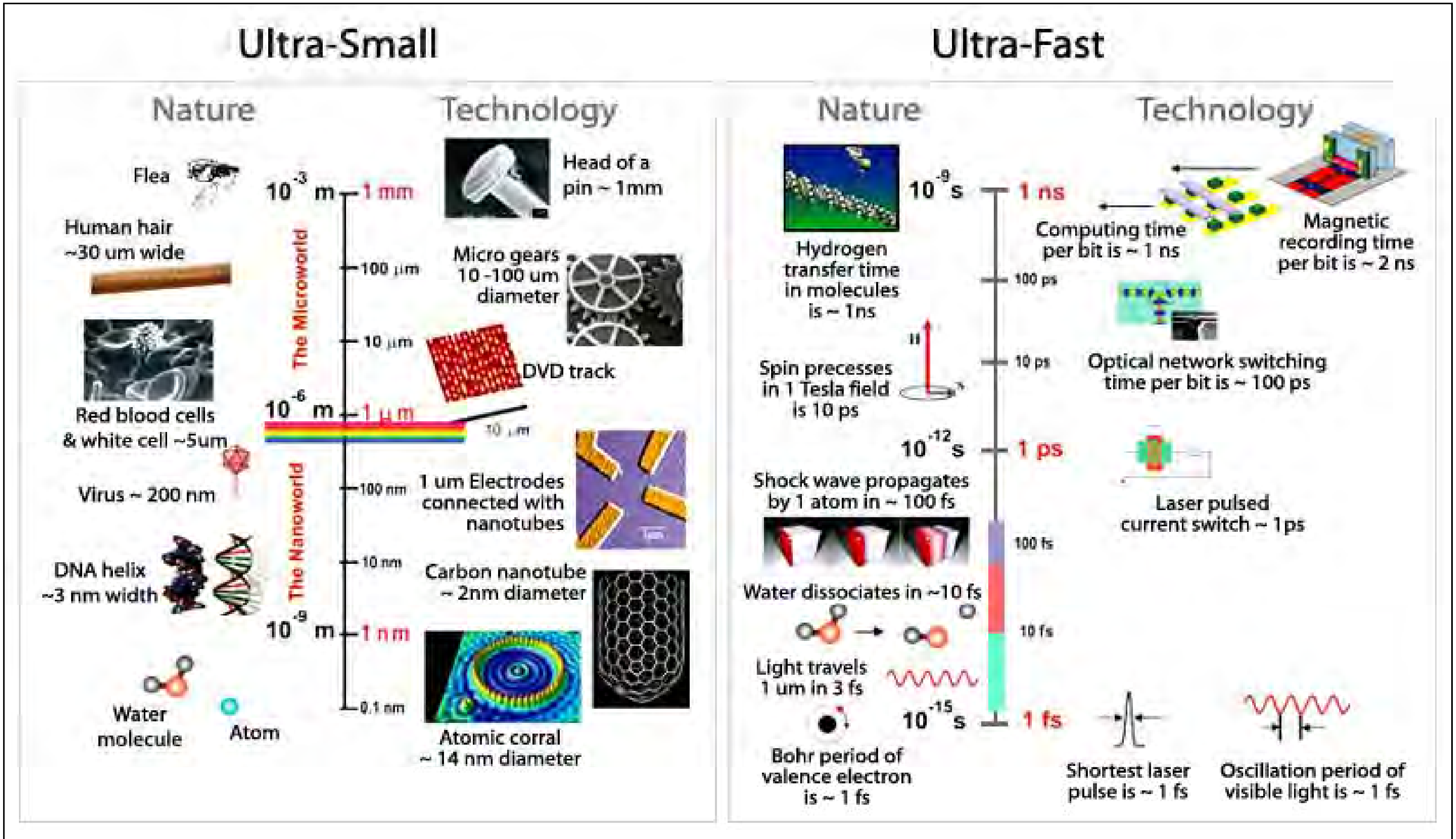
Molecular Foundry (Lawrence Berkeley National Laboratory)

Center for Functional Nanomaterials (Brookhaven National Laboratory)

Center for Nanophase Materials Sciences (Oak Ridge National Laboratory)

Center for Integrated Nanotechnologies (Sandia & Los Alamos National Labs)

Ultra-small and Ultra-fast: A Unified Theme for Research and Facilities



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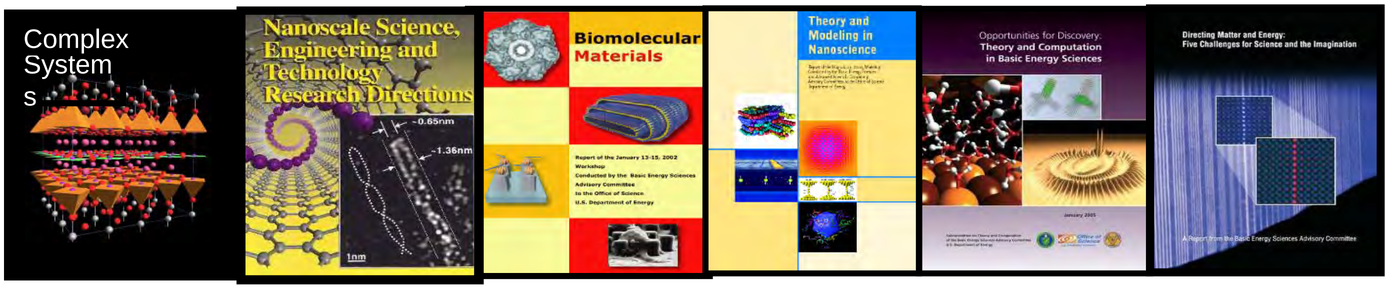
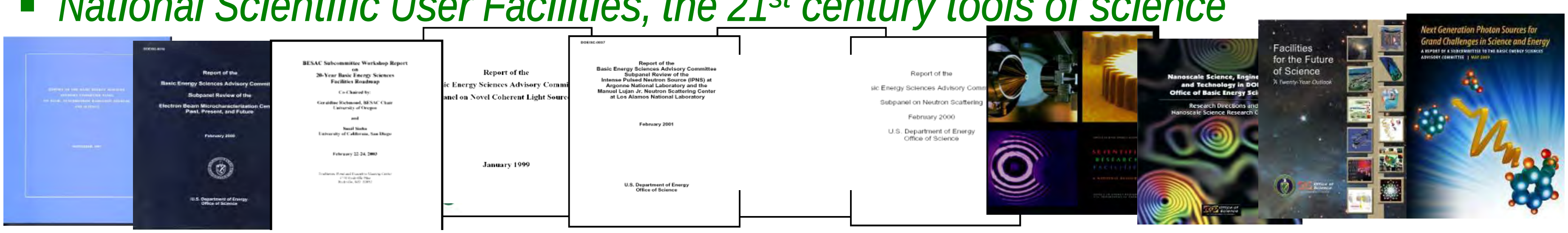
BESAC & BES Strategic Planning Activities

- *Science for Discovery*

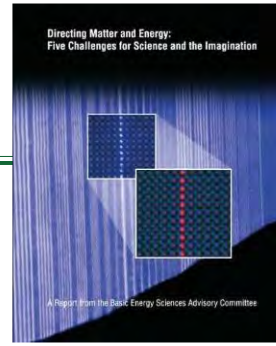


- *Science for National Needs*

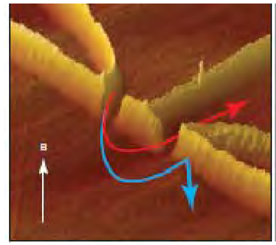
- *National Scientific User Facilities, the 21st century tools of science*



Science for Discovery -
Directing and Controlling Matter and Energy

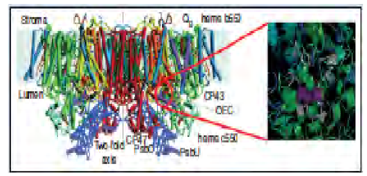


- Control the quantum behavior of electrons in materials
  Direct manipulation of the charge, spin, and dynamics of electrons to control and imitate the behavior of physical, chemical and biological systems, such as digital memory and logic using a single electron spin, the pathways of chemical reactions and the strength of chemical bonds, and efficient conversion of the Sun's energy into fuel through artificial photosynthesis.



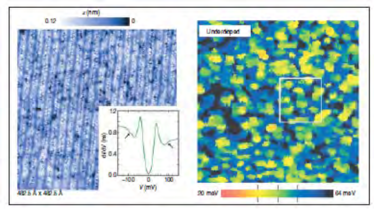
Atomic force micrograph of a device used to separate electrons according to their spin

- Synthesize, atom by atom, new forms of matter with tailored properties
  Create and manipulate natural and synthetic systems that will enable catalysts that are specific and produce no unwanted byproducts, or materials that operate at the theoretical limits of strength and fracture resistance, or that respond to their environment and repair themselves like those in living systems



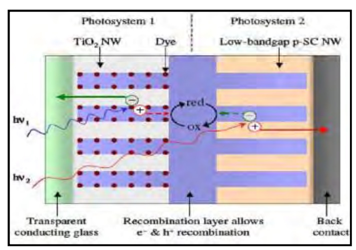
Structure of nature's photosynthetic membrane. The inset shows the manganese-based biological machine.

- Control emergent properties that arise from the complex correlations of atomic and electronic constituents
  Orchestrate the behavior of billions of electrons and atoms to create new phenomena, like superconductivity at room temperature, or new states of matter, like quantum spin liquids, or new functionality combining contradictory properties like super-strong yet highly flexible polymers, or optically transparent yet highly electrically conducting glasses, or membranes that separate CO_2 from atmospheric gases yet maintain high throughput.



(Left) Atomic-resolution scanning tunneling microscope image at 4.2K of BiSrCaCuO, (Right) A map of the superconducting gap.

- Synthesize man-made nanoscale objects with capabilities rivaling those of living things
  Master energy and information on the nanoscale, leading to the development of new metabolic and self-replicating pathways in living and non-living systems, self-repairing artificial photosynthetic machinery, precision measurement tools as in molecular rulers, and defect-tolerant electronic circuits



Tandem photovoltaics combine two systems for photon capture and charge separation, analogous to natural photosynthesis.

- Control matter very far away from equilibrium
  Discover the general principles describing and controlling systems far from equilibrium, enabling efficient and robust biologically-inspired molecular machines, long-term storage of spent nuclear fuel through adaptive earth chemistry, and achieving environmental sustainability by understanding and utilizing the chemistry and fluid dynamics of the atmosphere.

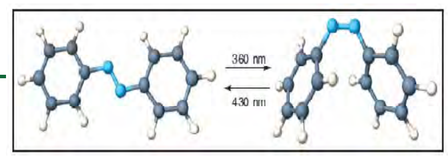


Photo-interconversion of two isomers of the azobenzene molecule. The direction of the interconversion depends on the wavelength of the light.

Science for National Need

Bringing forefront scientific knowledge and state-of-the-art tools to solving grand energy challenges

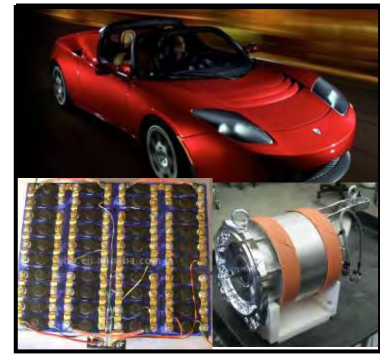
- Basic Research Needs for the Hydrogen Economy
- Basic Research Needs for Solar Energy Utilization
- Basic Research Needs for Superconductivity
- Basic Research Needs for Solid State Lighting
- Basic Research Needs for Advanced Nuclear Energy Systems
- Basic Research Needs for the Clean and Efficient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

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

BES Strategic Priorities

Energy Sustainability and Control Science

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



Greater Sustainability = Greater Complexity, higher functional materials

Basic and Applied R&D Coordination

How Nature Works … to … Design and Control … to … Technologies for the 21st Century

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

Discovery and

- 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

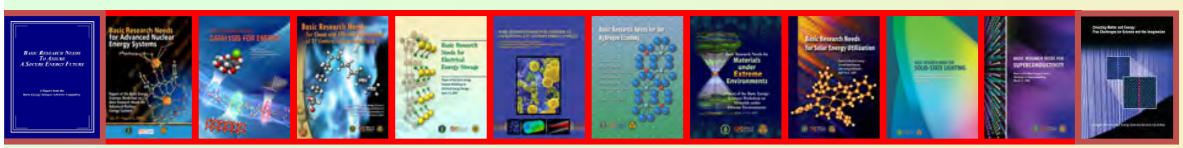
- Research with the goal of meeting *technical milestones*, with emphasis on the development, performance, cost reduction, and durability of materials and components or on efficient processes
- Proof of technology concepts

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

BESAC & BES Basic Research Needs Workshops

BESAC Grand Challenges Panel

DOE Technology Office/Industry Roadmaps



Energy Frontier Research Centers
Tackling Our Energy Challenges in a New Era of Science

EFRC awards provide the recipients with $2-5 million/year over a five-year award period to pursue collaborative basic research that addresses both energy challenges and science grand challenges in areas including:

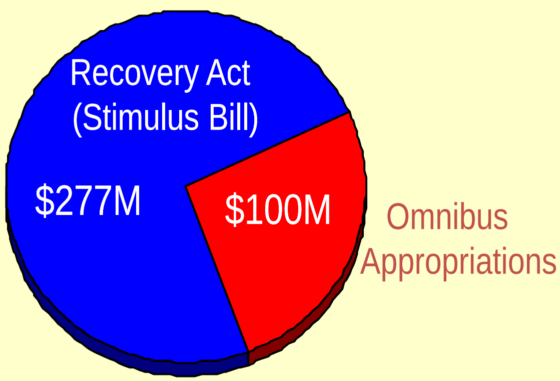
- Solar Energy Utilization
- Bio-Fuels
- Catalysis
- Energy Storage
- Geosciences for Waste and CO_2 Storage
- Advanced Nuclear Energy Systems
- Materials Under Extreme Environments
- Hydrogen
- Combustion
- Superconductivity
- Solid State Lighting

As stated in the Funding Opportunity Announcement for the EFRCs:

"… the research proposed in the EFRC application must:

1) address one or more of the challenges described in the BESAC report Directing Matter and Energy: Five Challenges for Science and the Imagination (http://www.sc.doe.gov/bes/reports/files/GC_rpt.pdf), and
2) address one or more of the energy challenges described in the 10 BES workshop reports in the Basic Research Needs series (http://www.sc.doe.gov/bes/reports/list.html)"

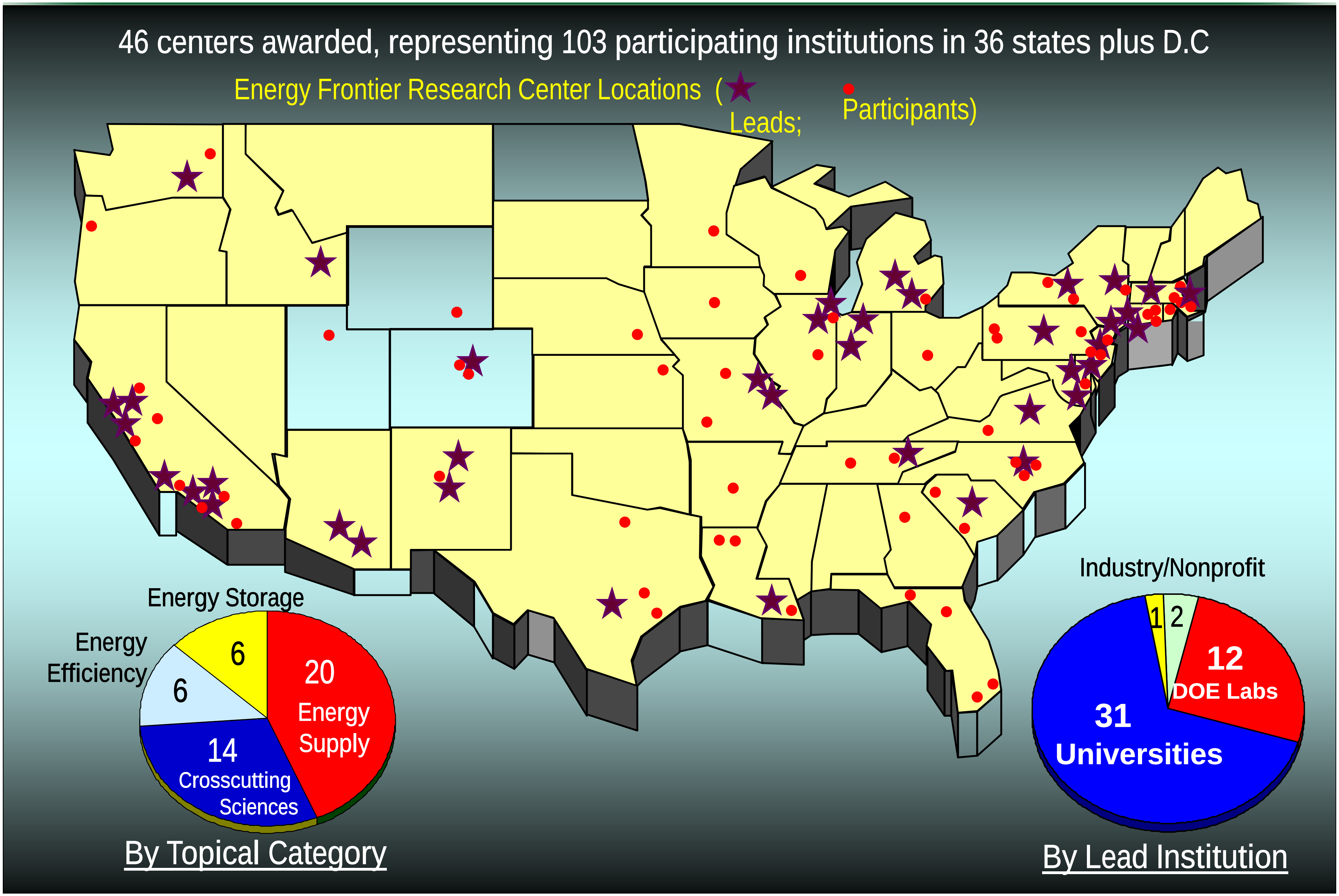
FY 2009 EFRCs Funding:



Total EFRCs = $777M over 5 years

The Status of the SC/BES Energy Frontier Research Centers

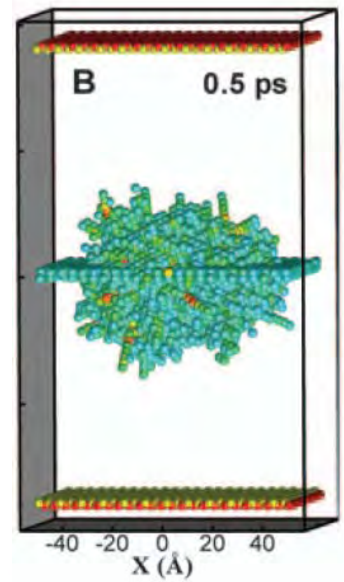
46 EFRCs were launched in late FY 2009 using FY 2009 Appropriations and Recovery Act Funds

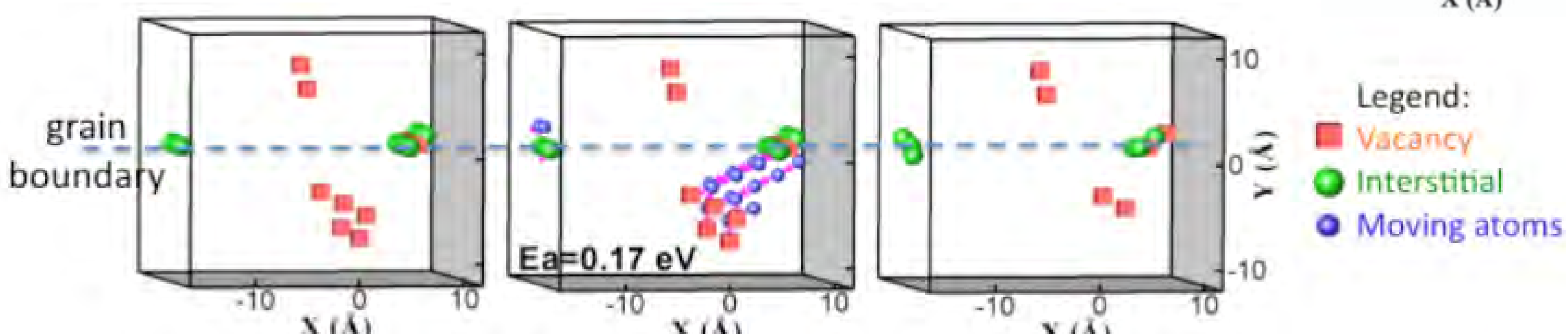


EFRC Highlight: Understanding Radiation Resistance in Materials

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

EFRC Highlight: Optimizing Light Absorption and Carrier Transport in Solar Cells

Energy Frontier Research Center on Light-Material Interactions in Energy Conversion

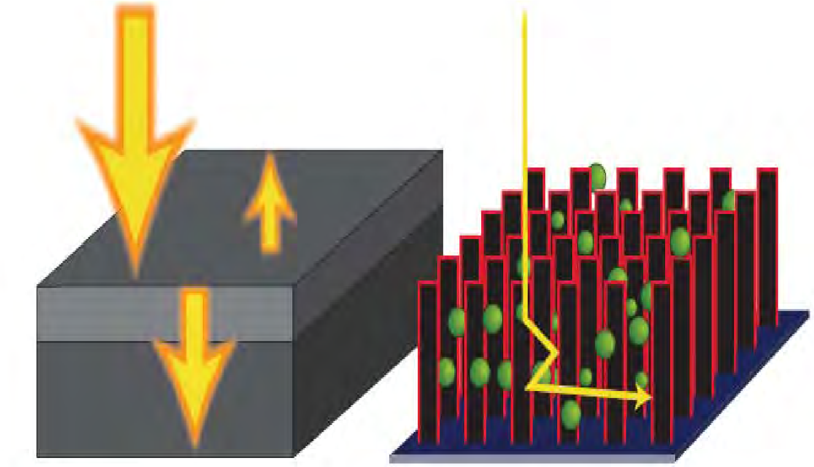
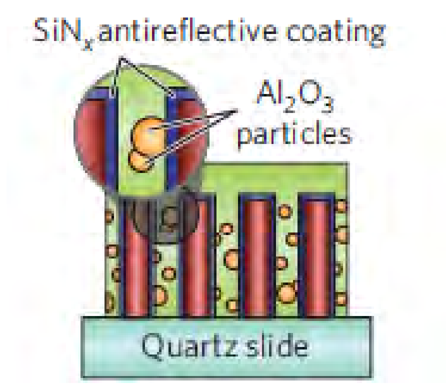


Figure 1 | Solar-cell light management. a, Conventional thin-film solar cells where incident light gets partially reflected. **b,** In the microwire arrays, Al_2O_3 nanoparticles (shown in green) reflect incident light and redirect it towards the micropillars.



- Simulations predict that light absorption and charge collection are optimal when the diameter of wires is on the order of the minority-carrier diffusion length, ca. 2 to 10 microns in low-purity silicon
- Based on this prediction, silicon solar cells were fabricated as follows:
  - Si wire arrays with these diameters and SiN_x antireflective coating
  - Arrays embedded in PDMS with 0.9 micron Al_2O_3 which redirect light towards micropillars

    Arrays can be peeled off and put on flexible substrate
- Absorb up to 85% of the sunlight but fills as little as 1% of the cell's volume and uses only 1/100th of the Si in a conventional cell.
- Potential for increased photovoltaic efficiency owing to an effective optical concentration of up to 20 times.

U.S. DEPARTMENT OF ENERGY | Office of Science

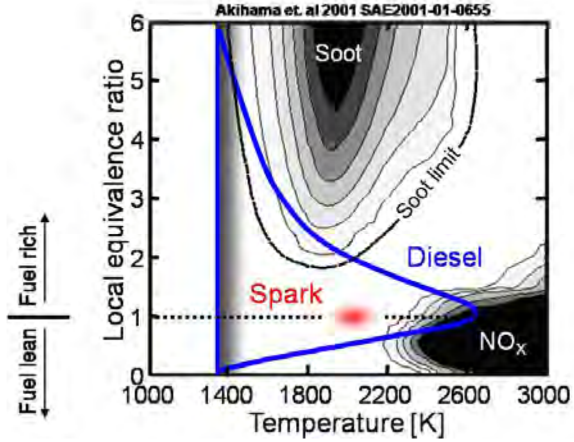
Performers: Nathan Lewis and Harry Atwater, California Institute of Technology-EFRC
Publication: M. D. Kelzenberg, et al. *Nature Materials*, **2010**, *9*, 239-244.

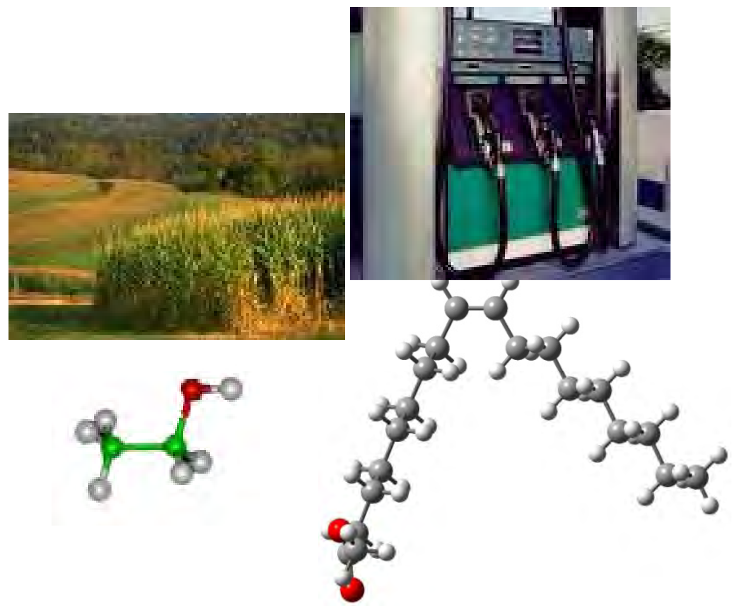
The Science Base for Multi-Scale Simulation of Internal Combustion Engines-

A New Initiative in FY 2011

Transportation Combustion Challenge: How to get "clean" and "efficient"?

- Transportation accounts for 60% of oil consumption
- Combustion engine viable for decades to come, but efficiency & cleanliness difficult to achieve together
- Fuel streams are rapidly evolving
  - Heavy hydrocarbons: oil sands, oil shale, coal
  - New renewable fuel sources: ethanol, biodiesel
- New engine technologies
  - Direct Injection (DI)
  - Homogeneous Charge Compression Ignition (HCCI)
  - Low-temperature combustion
- Hybrid vehicle technologies

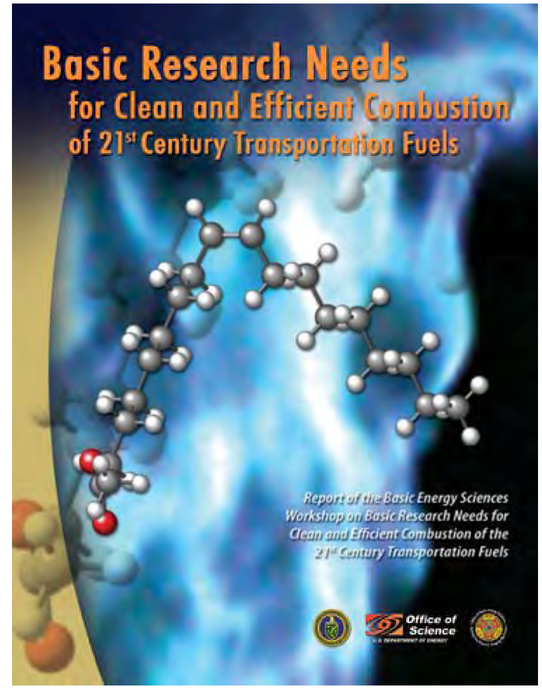




Multi-scale Simulation of Internal Combustion Engines

A new initiative to develop the science base for computational design of advanced engines

Predictive simulation of combustion in an evolving fuel environment is essential for developing more efficient and cleaner engines.



The scientific community has provided a roadmap via:

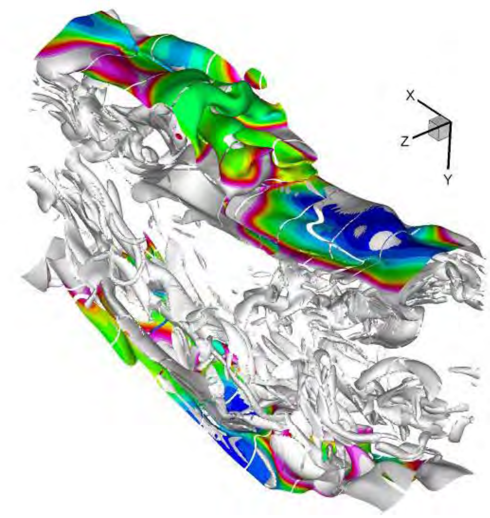
- BES workshop: *Basic Research Needs for Clean and Efficient Combustion*, October 2006
- ASCR/BES workshop: *Discovery in Basic Energy Sciences: The Role of Computing at the Extreme Scale*, August 2009
- SC ongoing collaboration with EERE's Vehicle Technology Program

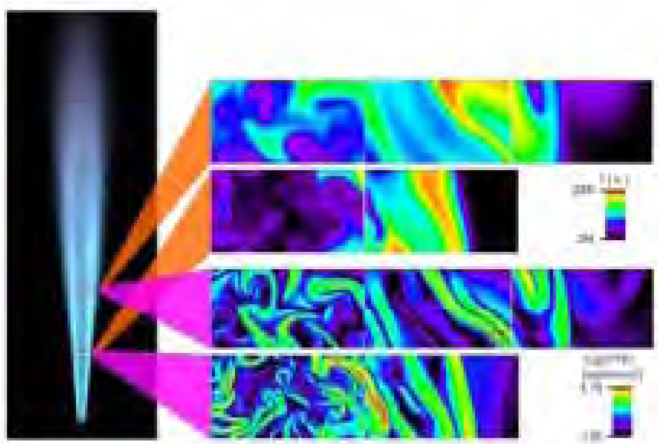
The new BES activity (+$20,000K) will provide:

- Models that span vast scale ranges: coupling of combustion chemistry with turbulent flow requiring simulation over 9 orders of magnitude in space and time.
- Improved understanding of fundamental physical and chemical properties: multi-phase fluid dynamics, thermodynamic properties, heat transfer, and chemical reactivity.
- Engine simulation: science-based predictive simulation and modeling design

Establishing the science base for multi-scale simulation of advanced engines

- Computational chemistry and benchmark combustion simulations (in collaboration with ASCR).
  - **Numerical investigations of canonical flame behavior**
  - **Automated discovery of chemical reaction mechanisms and kinetics**
- Experimental validation, verification, and discovery.
  - **Cinematic imaging of canonical flames**
  - **Mulitplex investigation of chemical reactions**
- To set the stage for subsequent development of new, science-based engineering tools for advanced engine design (in collaboration with EERE Vehicle Technologies Program).





Top: Direct numerical simulation of a CO/H2 slot flame
Bottom: Imaging of a model flame jet flame