U.S. Department of Energy

Office of Science

U.S. Department of Energy
Office of Science

Basic Research for Our Nation's Energy Future

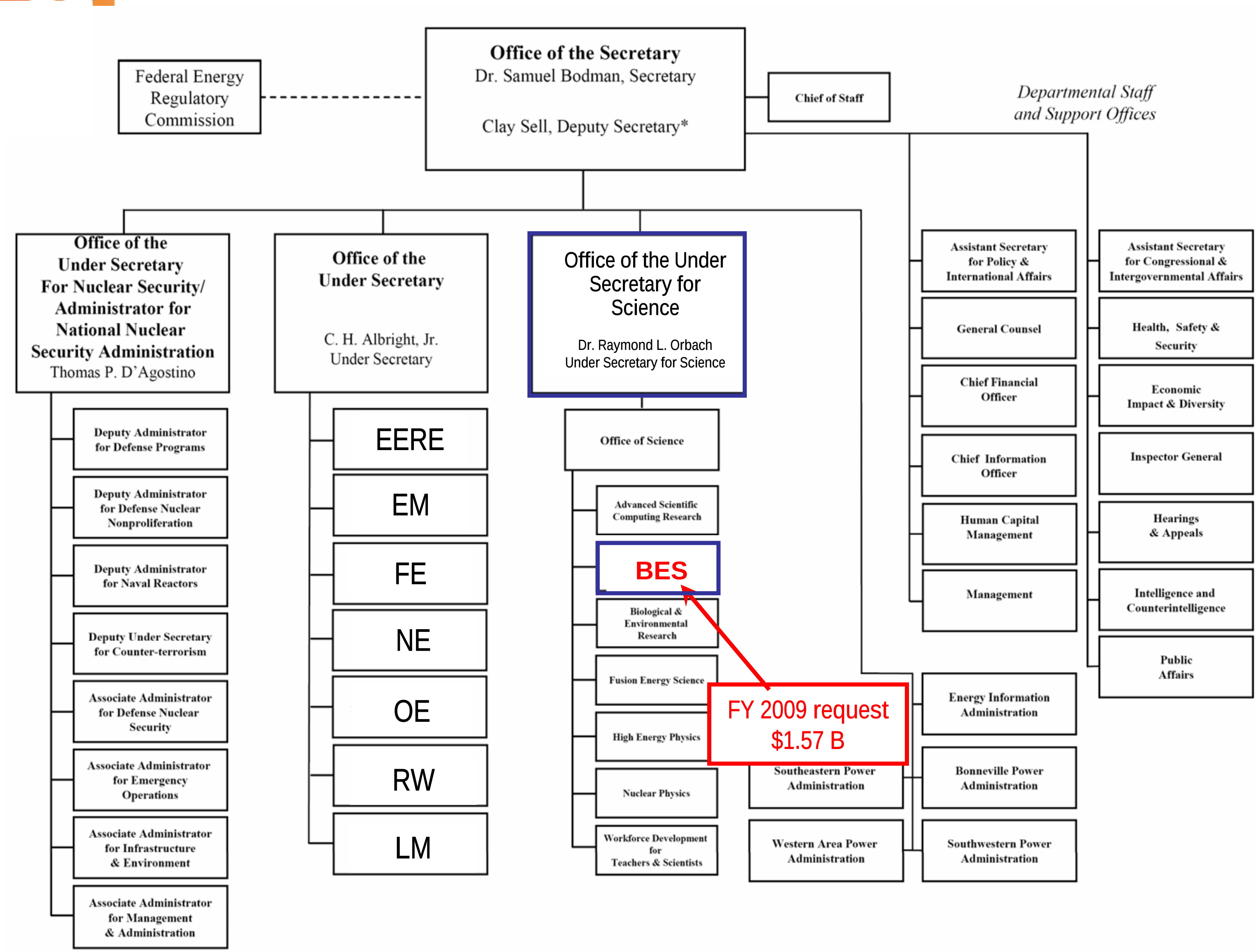
John S. Vetrano
Program Manager
Office of Science
Office of Basic Energy Sciences

VC Technology Commercialization Showcase

August 6, 2008

John.vetrano@science.doe.gov

Department of Energy



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

Grand Challenges
How nature works

- 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
Materials properties and functionalities by design

- 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

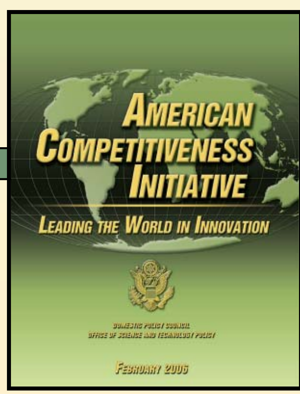
Technology Maturation & Deployment

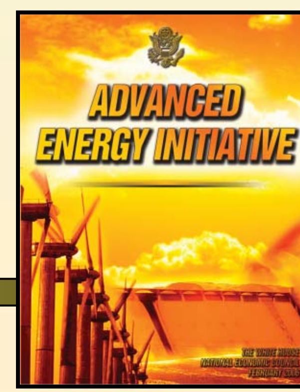
- Scale-up research
- At-scale demonstration
- Cost reduction
- Prototyping
- Manufacturing R&D
- Deployment support

BESAC & BES Basic Research Needs Workshops

BESAC Grand Challenges Panel

DOE Technology Office/Industry Roadmaps





U.S. Department of Energy

Office of Science

Office of Basic Energy Sciences

Harriet Kung, Director

- BES Budget and Planning
- BES Operations

Materials Sciences and Engineering Division

Arvind Kini, Acting Director

- Materials Discovery, Design, and Synthesis
  - Materials Chemistry
  - Biomolecular Materials
  - Synthesis and Processing
  - Tech. Coordination Program Management
- Condensed Matter and Materials Physics
  - Experimental Condensed Mat. Physics
  - Theoretical Condensed Matter Physics
  - Physical Behavior of Materials
  - Mechanical Behavior and Radiation Effects
- Scattering & Instrumentation Sciences
  - X-ray Scattering
  - Neutron Scattering
  - Electron and Scanning Probe Microscopies
  - Ultrafast Science and Instrumentation
  - Exp. Program to Stimulate Competitive Research

Scientific User Facilities Division

Pedro Montano, Director

- Operations
  - X-ray and Neutron Scattering Facilities
  - Nanoscience Centers & E-beam Centers
  - Accelerator and Detector R&D
  - Facility Coordination, Metrics, Assessment
- Construction
  - Linac Coherent Light Source
  - NSLS II
  - Spallation Neutron Source Upgrades
  - TEAM
  - Instrument MIEs (SING, LUSI, etc.)
  - ALS User Support Bldg

Chemical Sciences, Geosciences, and Biosciences Division

Eric Rohlfing, Director

- Fundamental Interactions
  - Atomic, Molecular, and Optical Sciences
  - Gas-Phase Chem. Phys.
  - Condensed-phase and Interfacial Mol. Sci.
  - Computational and Theoretical Chemistry
- Photo- and Bio-Chemistry
  - Solar Photochemistry
  - Photosynthetic Systems
  - Physical Biosciences
- Chemical Transformations
  - Catalysis Science
  - Heavy Element Chemistry
  - Separations and Analysis
  - Geosciences
  - Technology Office Coordination

Office of Basic Energy Sciences

Our Mission:

- Foster and support ***fundamental research programs*** to expand the scientific foundation for new and improved energy technologies and for understanding and mitigating the environmental impacts of energy use

- Plan, construct, and operate ***major scientific user facilities*** for "materials sciences and related disciplines" to serve researchers at universities, federal laboratories, and industrial laboratories

BES Research Portfolio

Distinguishing Features:

- Idea-driven fundamental research
- Underpin broadly-defined energy missions
- Addressing long-range grand challenges
- Scientific excellence and innovation
- Revolutionary and high risk-high payoff approaches
- Strive for flexibility and stability
- Competitive and peer review process

Deliverables:

- Knowledge broadly disseminated
- High impact results/publications
- New concepts/design for instrumentation
- Important discoveries impacting others' research

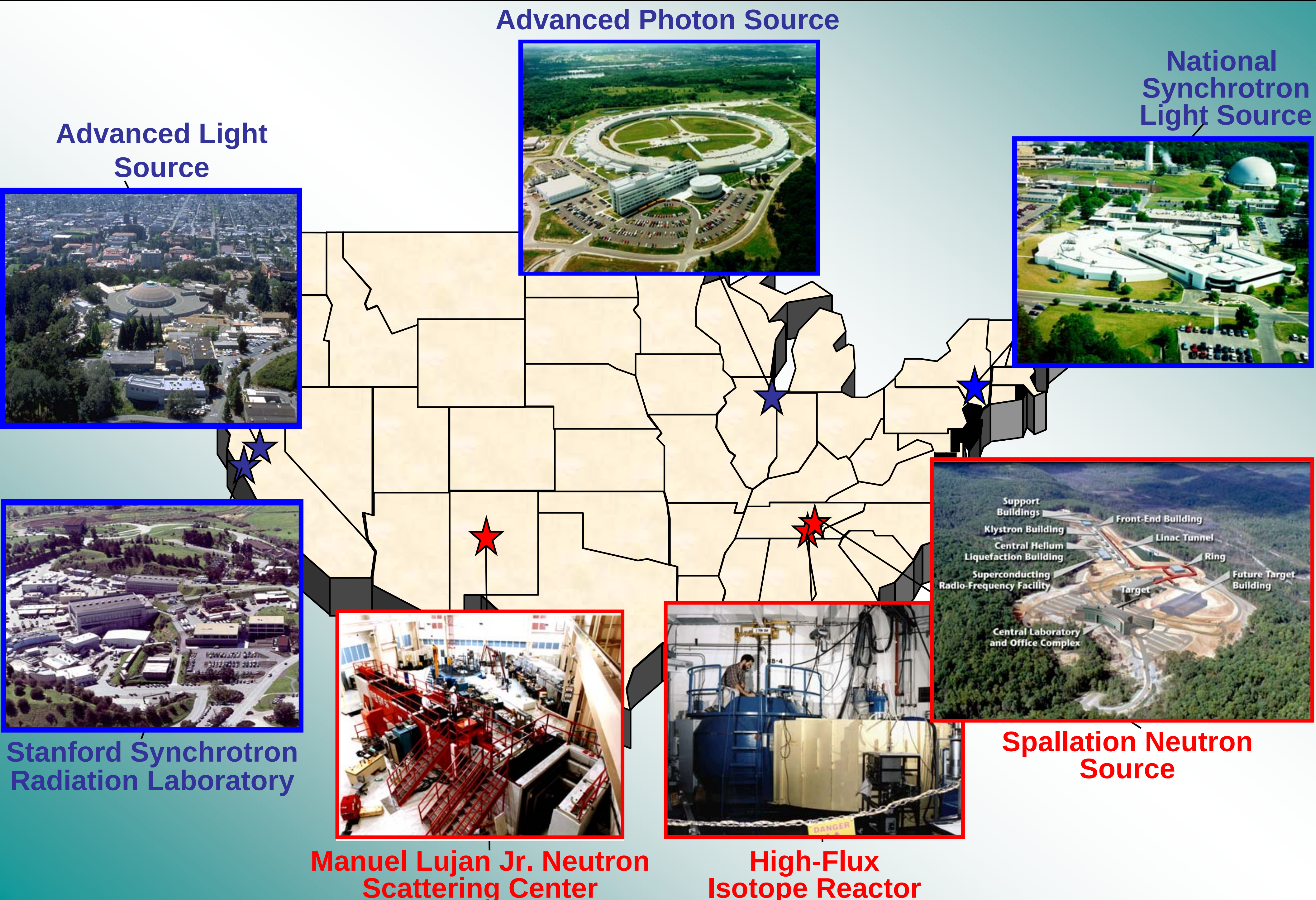
Serving the Present, Shaping the Future

Impacting directions in basic and applied research and technology development

The five NanoScience Research Centers are in operations and serving users

BES Neutron and X-ray Scattering User Facilities

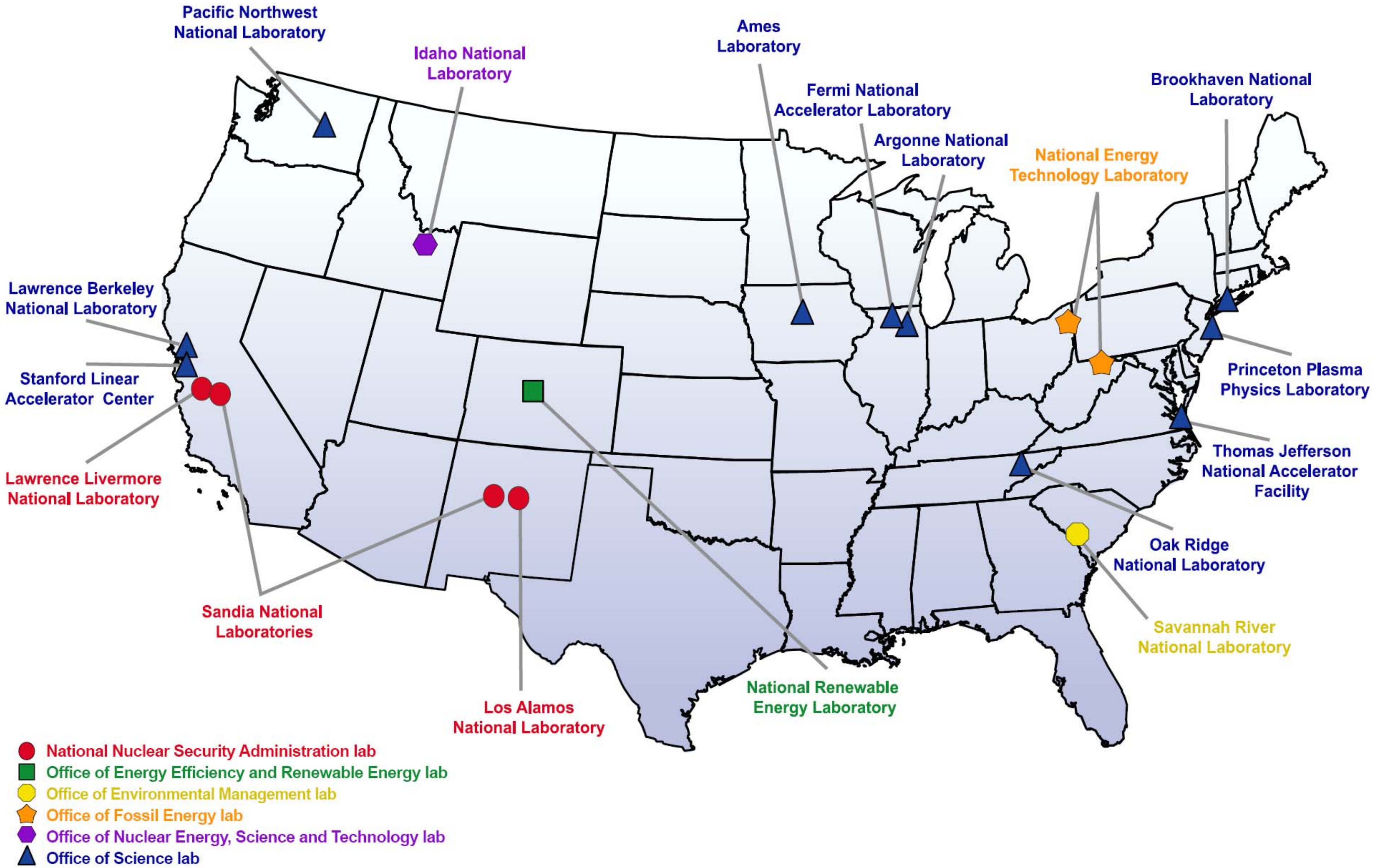
Characterizing Nanoscale Materials for Energy Applications



U.S. Department of Energy

Office of Science

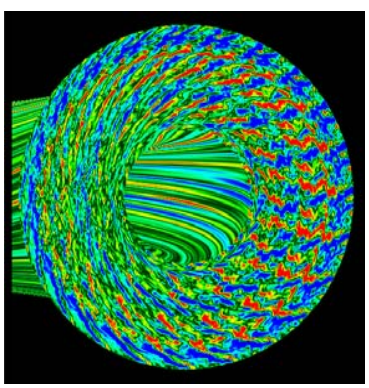
Department of Energy National Laboratories



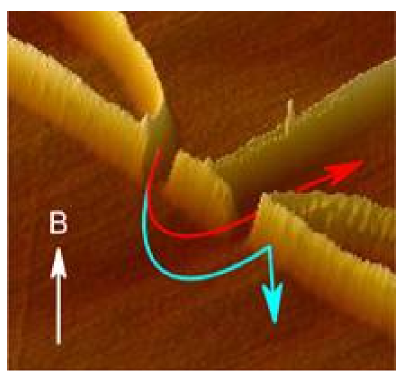
The Essential Role of Basic Science

Incremental changes in current technologies will not suffice; transformational changes are needed.

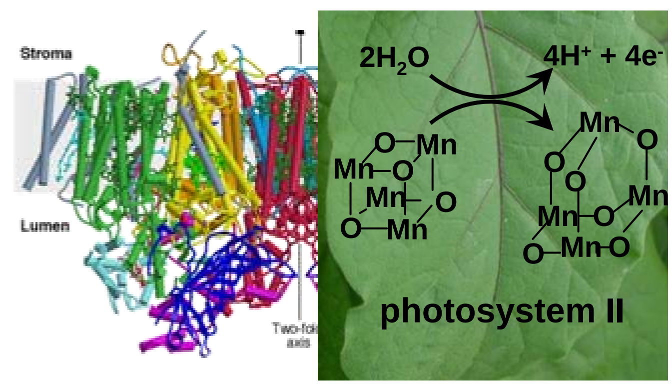
- Today's energy technologies and infrastructure are rooted in 20th Century technologies and 19th Century discoveries—internal combustion engine, electric lighting, alternating current.
- Current fossil energy sources, current energy production methods, and current technologies cannot meet the energy challenges we now face.
- Incremental changes in technology will not suffice. We need **transformational discoveries** and truly **disruptive technologies.**
- 21st Century technologies will require the ability to direct and control matter down to the molecular, atomic, and quantum levels.



Computer simulation of plasma turbulence in a tokamak



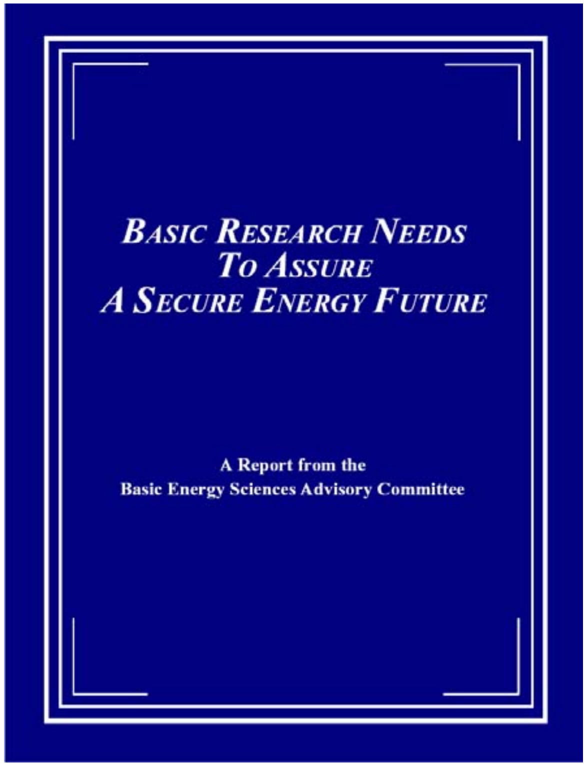
Separating electrons by their spin for "spintronics" and other applications of electron control.



Bio-inspired nanoscale assemblies – self-repairing and defect-tolerant materials and selective and specific chemical reactivity.

The First "Basic Research Needs ..." Workshop

Basic Research Needs to Assure a Secure Energy Future (October 2002)



- The report identified basic research directions required for major technological changes in the largest industries in the world—those responsible for energy production and use.
- The reports highlighted the remarkable scientific journey that took place during the past few decades. The resulting scientific challenges describe a new era of science — an era in which materials functionalities are designed to specifications and chemical transformations are manipulated at will.
- In this new era of science, we design, discover, and synthesize new materials and molecular assemblies through atomic scale control; probe and control photon, phonon, electron, and ion interactions with matter; perform multi-scale modeling that bridges the multiple length and time scales; and use the collective efforts of condensed matter and materials physicists, chemists, biologists, molecular engineers, applied mathematicians, and computer scientists.
- The findings inspired 10 additional workshops over the next five years, which together attracted more than 1,500 participants.

The Workshop Set Forth 37 Research Directions

Topics covered energy supply, conversion, storage, distribution, efficiency , and end use

Fossil Energy

- Reaction pathways of inorganic solid materials: synthesis, reactivity, stability
- Advanced subsurface imaging and alteration of fluid-rock interactions
- Development of an atomistic understanding of high-temperature hydrogen conductors
- Fundamental combustion science towards predictive modeling of combustion technologies

Renewable and Solar Energy

- Displace imported petroleum by increasing the cost-competitive production of fuels and chemicals from renewable biomass by a hundred fold
- Develop methods for solar energy conversion that result in a ten-to-fifty fold decrease in the cost-to-efficiency ratio for the production of fuels and electricity
- Develop the knowledge base to enable widespread creation of geothermal reservoirs
- Conversion of solar, wind, or geothermal energy into stored chemical fuels
- Advanced materials for renewable energy applications

Bioenergy

- Energy biotechnology: metabolic engineering of plants and microbes for renewable production of fuels and chemicals
- Genomic tools for the development of designer energy and chemical crops
- Nanoscale hybrid assemblies for the photo-induced generation of fuels and chemicals

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

Distributed Energy, Fuel Cells, and Hydrogen

- Advanced hydrogen synthesis
- High-capacity hydrogen storage for distributed energy of the future
- Novel membrane assemblies
- Designed interfaces

Residential, Commercial, and Industrial Energy Consumption

- Sensors
- Solid state lighting
- Innovative materials for new energy technologies
- Multilayer thin film materials and deposition processes

Transportation Energy Consumption

- Integrated quantitative knowledge base for joining of lightweight structural materials for transportation applications
- Vehicular energy storage
- Fundamental challenges in fuel cell stack materials
- Integrated heterogeneous catalysis
- Thermoelectric materials and energy conversion cycles for mobile applications
- Complex systems science for sustainable transportation

Cross-Cutting Research and Education

- Nanomaterials
- Preparing tomorrow’s workforce for the energy challenge and heightening the public’s awareness

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

U.S. Department of Energy

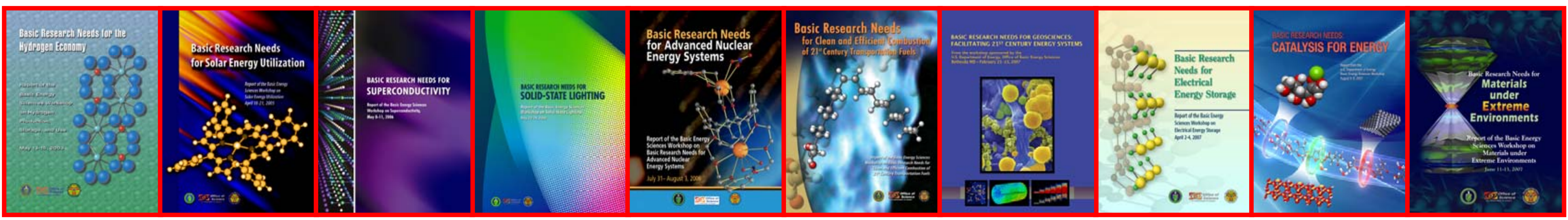
Office of Science

The 10 "Basic Research Needs …" Workshops

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

Basic Research Needs to Assure a Secure Energy Future (BESAC)

- 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

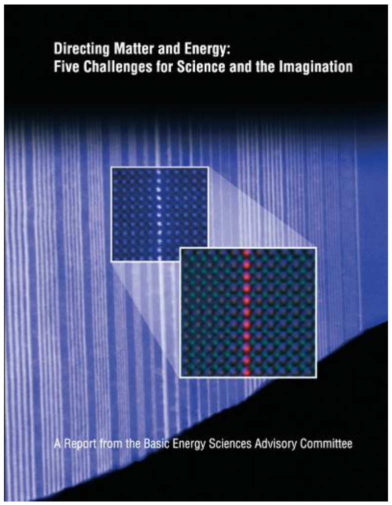


www.science.doe.gov/bes/reports/list.html

One Additional Workshop: Science Grand Challenges

How does nature execute electronic and atomic design? How can we?

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



- Control the quantum behavior of electrons in materials
  Imagine: 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
- Synthesize, atom by atom, new forms of matter with tailored properties
  Imagine: Create and manipulate natural and synthetic systems that will enable catalysts that are 100% 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
- Control emergent properties that arise from the complex correlations of atomic and electronic constituents
  Imagine: 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.
- Synthesize man-made nanoscale objects with capabilities rivaling those of living things
  Imagine: 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
- Control matter very far away from equilibrium
  Imagine: 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

How Nature Works … to … Materials 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 *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

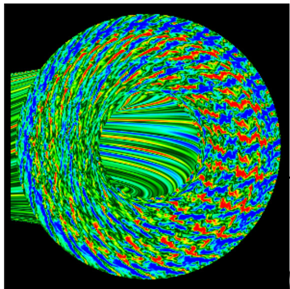
DOE Technology Office/Industry Roadmaps

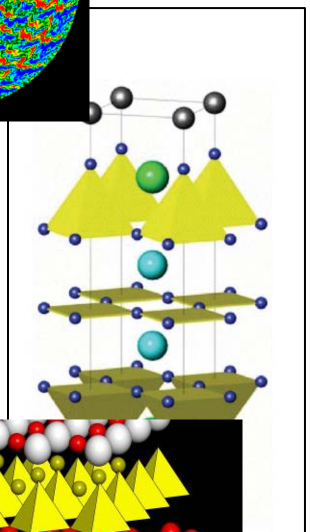
BES Energy Frontier Research Centers

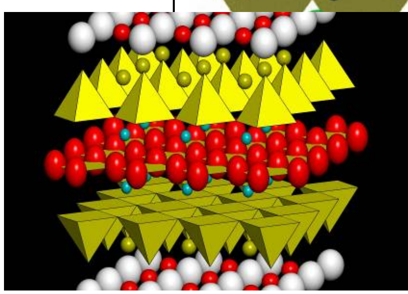
Tackling our Energy Challenges in a New Era of Science

Science Transforming Energy Technologies

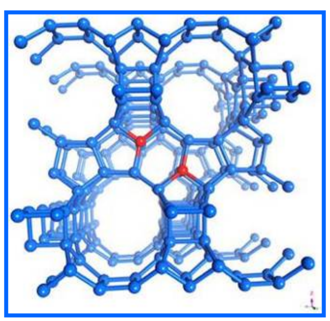
Examples in energy supply, conversion, storage, distribution, and end use



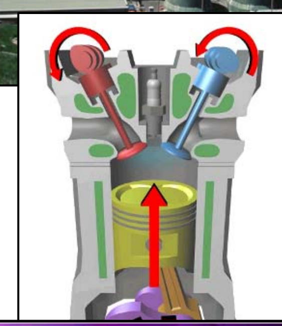




High Tc super-conductors



- Solar energy utilization
- Biofuels production
- Advanced nuclear energy systems
- Combustion of transportation fuels
- Electrical energy storage
- Hydrogen production, storage, and use
- Superconductivity
- Solid state lighting
- Catalysis for energy applications
- Materials under extreme environments
- Geosciences

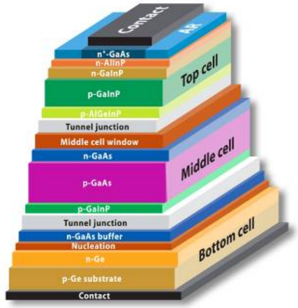


Solar Energy

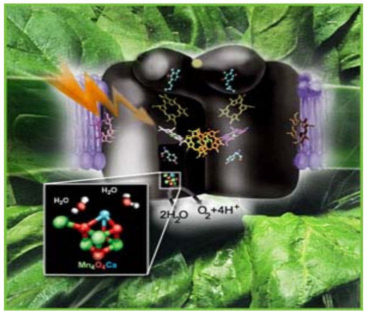
Science Transforming Energy Technologies

Imagine:
- Solar photovoltaics exceeding thermodynamic efficiency limits
- Direct conversion of sunlight to chemical fuels

- Sunlight provides by far the largest of all carbon-neutral energy sources – more energy from sunlight strikes the Earth in one hour (4.6 x 10^{20} joules) than all the energy consumed on the planet in a year.
- Despite the abundance, less than 0.1% of our primary energy derives from sunlight.
- The three routes for using solar energy – conversion to electricity, fuels, or thermal heat – exploit the functional steps of capture, conversion, and storage. They also exploit many of the same electronic and molecular mechanisms.
- The challenge: reducing the costs and increasing the capacity of converting sunlight into electricity or fuels that can be stored or transported (solar electricity, solar fuels, solar thermal systems).
- Silicon: The top commercial solar cells (single crystal silicon) have reached conversion efficiencies of 18%; triple-junction cells with Fresnel lens concentrator technology are approaching efficiencies of 40%. Cost-effective improvements in efficiency dependent on our ability to understand and control phenomena at the nanoscale.
- Photosynthesis: Borrowing nature's design for capturing sunlight – bio-inspired nanoscale assemblies to produce fuels from water and CO_2.



A multi-layered triple-junction solar cell designed to absorb different solar photons.



Photosystem II uses solar energy to break two molecules of water into one oxygen molecule plus four hydrogen ions, meanwhile freeing electrons to drive other reactions.

Basic Research Needs for Solar Energy Utilization

The physical, chemical, and biological pathways of solar energy conversion meet at the nanoscale. The ability to create nanoscale structures coupled with advanced characterization, theory, and computational tools suggest that understanding and control of efficient solar energy conversion are within reach.

- Photovoltaics exceeding thermodynamic efficiency limits

  New concepts, structures, and methods of capturing the energy from sunlight without thermalization of carriers are required to break through the Shockley-Queisser efficiency barrier (32%). Multiple-exciton generation from a single photon is a prime example.

- Easily manufactured, low-cost polymer and nanoparticle photovoltaic structures

  "Plastic" solar cells made from molecular, polymeric, or nanoparticle-based structures could provide flexible, inexpensive, conformal solar electricity systems.

- Efficient photoelectrolysis

  Solar fuels generation involves coupling photo-driven single electron steps with fuel-forming, multi-electron processes. No man-made systems approach the performance of naturally found enzymes. Practical solar fuel formation requires construction of new catalyst systems to form hydrogen and oxygen from water and to efficiently reduce carbon dioxide from the air.

- Defect-tolerant and self-repairing systems

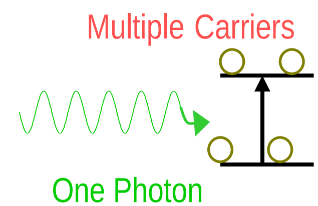
  Understanding the defect formation in photovoltaic materials and self-repair mechanisms in photosynthesis will lead to defect tolerance and active self-repair in solar energy conversion devices, enabling 20+ years operation.

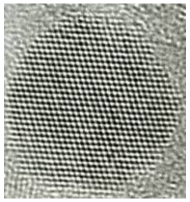
- Bio-inspired molecular assemblies systems

  The design and development of light-harvesting, photoconversion, and catalytic modules capable of self-ordering and self-assembling into an integrated functional unit to realize an efficient artificial photosynthetic system for solar fuels.

- New experimental and theoretical tools

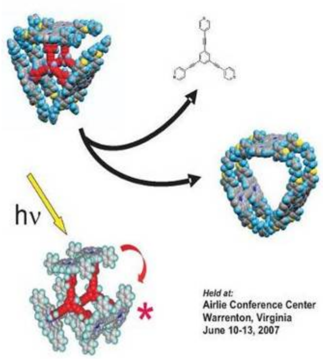
  Tools that could enable the theoretical prediction of optimally performing structures.





Si nano-crystals (7 nm dia-meter)

Multiple exciton generation in Si quantum dots



A prism-shaped assembly of three porphyrin molecules that displays enhanced light harvesting capability

Bioenergy

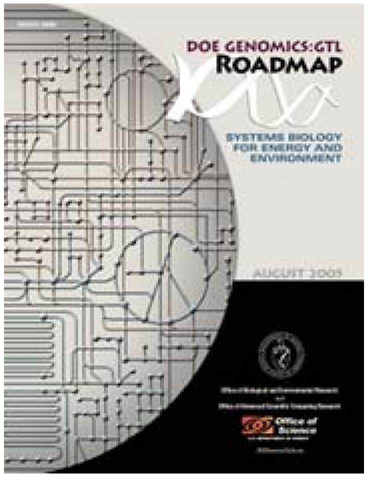
Science Transforming Energy Technologies

Imagine:
- Sustainable, carbon-neutral biofuels meeting > 30% of U.S. transportation fuel needs (cars and trucks) without competing with food, feed, or export demands

- The development of biofuels—especially lignocellulose biofuels—represents a major scientific opportunity that can strengthen U.S. energy security and protect the global environment.
- Biofuels can be essentially carbon-neutral or even carbon-negative – as plant feedstocks grow, they reabsorb the carbon dioxide emitted when biofuels are burned, and they can store carbon dioxide in their roots.
- To produce lignocellulosic biofuels, or biofuels from plant fiber, cost-effectively on a commercial scale will require transformational breakthroughs in basic science focused on both plants and microorganisms and processing methods.
- The challenge is the recalcitrance of the plant cell wall – plant fiber has evolved over the millennia to be extremely resistant to breakdown by biological or natural forces.
- Many scientists believe we are within reach of major breakthroughs in developing cost-effective methods of producing liquid fuels from lignocellulose in the near- to mid- term.
- The environmental sustainability aspects associated with bioenergy derived from feedstock crops – water, soil quality, land-use changes, genetically altered plants, carbon balance – must be addressed proactively.

Biotechnology offers the promise of dramatically increasing ethanol production using cellulose and other polysaccharides (hemicellulose). Residue including postharvest corn plants (stover) and timber residues could be used, as well as such specialized high-biomass "energy" crops as domesticated poplar trees and switchgrass.

DOE Bioenergy Research Centers

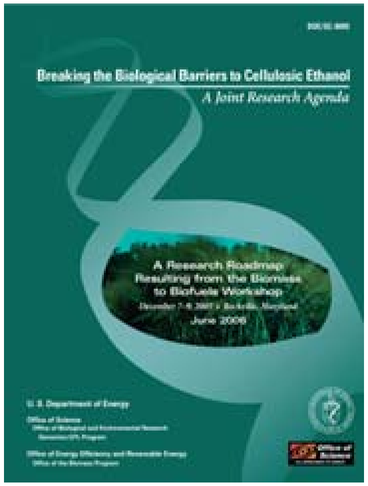


Grand Science Challenges:

- Using a systems biology approach, understand the principles underlying the structural and functional design of living systems — plants and microorganisms.
- Develop the capability to model, predict, and engineer optimized enzymes, microorganisms, and plants — bioenergy and environmental applications.

Research needed for cellulosic ethanol (and other biofuels) production:

The emerging tools of systems biology are being used to help to overcome current obstacles to bioprocessing cellulosic feedstocks to ethanol and other biofuels– metagenomics, synthetic biology, high-throughput screening, advanced imaging, high-end computational modeling.



- **DOE BioEnergy Science Center** – led by Oak Ridge National Laboratory, includes 9 partnering institutions. This center focuses on the resistance of plant fiber to breakdown into sugars and is studying the potential energy crops poplar and switchgrass.
- **DOE Great Lakes Bioenergy Research Center** – led by University of Wisconsin-Madison in partnership with Michigan State University, includes 6 other partnering institutions. This center is studying a range of plants and is exploring plant fiber breakdown and how to increase plant production of starches and oils, which are more easily converted to fuels. This Center also focuses on sustainability, examining the environmental and socioeconomic implications of moving to a biofuels economy.
- **DOE Joint BioEnergy Institute** – led by Lawrence Berkeley National Laboratory, includes 5 other partnering institutions. This center focuses on "model" crops of rice and *Arabidopsis thaliana* in the search for breakthroughs in basic science and is exploring microbial-based synthesis of fuels beyond ethanol.

Nuclear Energy

Science Transforming Energy Technologies

Imagine:
- Abundant fossil-free power with zero greenhouse gas emissions
- A closed fuel cycle

- Good for both energy security and the environment:
  - Reduces nation's dependence on fossil fuels and imports
  - No carbon dioxide or toxic emissions
- Currently provides 20% of nation's electricity and could provide much more
- Key challenge is handling spent fuel – and related problem of proliferation
- Advances in science and engineering can provide major reduction in spent fuel by "closing" fuel cycle:
  - Recycling spent fuel and burning it in fission reactors
  - Reducing storage requirements by up to 90%
  - Extending fuel supplies 100X; energy remaining in "spent" fuel
  - New recycling technologies could reduce nuclear materials proliferation concern

Performance of materials and chemical processes under extreme conditions is a limiting factor in all areas of advanced nuclear energy systems

Basic Science for Advanced Nuclear Energy Systems

Fundamental Challenge: To understand and control chemical and physical phenomena in complex systems from femto-seconds to millennia, at temperatures to 1000 ^{o}C, and for radiation doses to hundreds of displacements per atom.

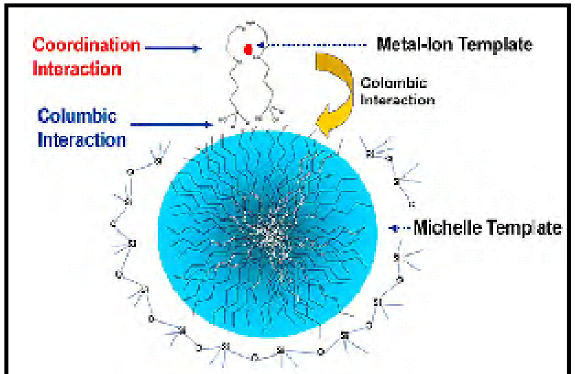
Basic Science:

- Research in Basic Energy Sciences
  - Materials and chemistry under extreme temperature, pressure, corrosive, and radiative environments; chemistry at interfaces and in complex solutions; separations science; advanced actinide fuels; nanoscale synthesis and characterization for design of materials and interfaces with radiation, temperature and corrosion resistence; predictive modeling and simulation
  - Workshop: Basic Research Needs for Advanced Nuclear Energy Systems, July 31-August 2, 2006.
- Research in Nuclear Physics
  - Nuclear measurements (neutron and charged particle beam accelerator experiments, cross-section measurements), nuclear data (cross-section evaluation, actinide nuclear data), nuclear theory and computation
  - Workshop: Nuclear Physics and Related Computational Science R&D for Advanced Fuels Cycles Workshop, August 10-11, 2006.
- Research in Advanced Scientific Computing
  - Developing and scaling next-generation multiscale and multiphysics codes; advanced modeling and simulation to improve future reactor designs; reactor core simulations; fluid flow and heat transfer; and radiation induced microstructural evolution of defects.
  - Workshop: Simulation and Modeling for Advanced Nuclear Energy Systems, August 15-17, 2006.

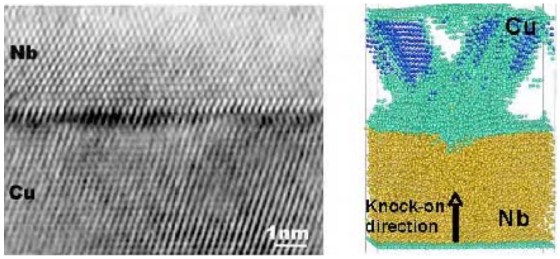
Basic Research Needs for Advanced Nuclear Energy Systems

Understand and control chemical and physical phenomena in multi-component systems requires bridging the scales from femtoseconds to millennia, at temperatures to 1000°C, and radiation doses to hundreds of dpa.

- Mastering the chemistry and physics of actinides and actinide-bearing materials (the *f*-electron challenge)
  - Theoretical development to address strong correlations, spin-orbit corrections, and relativistic effects and thereby obtain a sound, first-principles description of the electronic structure of actinide elements.
  - Predictive models of thermodynamics, phase equilibria, and kinetics of complex actinide mixtures as a function of temperature and irradiation fluence, coupled with experimental breakthroughs required to underpin our theoretical understanding of these *f*-electron materials and their compounds.
- Developing a first principles, multiscale description of material properties in complex materials under extreme conditions
  - Understand the mechanisms limiting the performance of structural materials at high temperature during irradiation, including the deleterious effects of high-dose irradiation on mechanical properties.
  - Extend current first-principles and atomistic and phase field models to fully describe irradiation-induced microstructural evolution in metallic alloys and complex interfaces.
  - Characterize the radiation-induced phenomena, interfacial phenomena, and effects of chemical composition changes evolving from radioactive decay processes to predict the long-term stability and chemical behavior of complexes of fission products and actinides in waste-form matrices.
- Understanding and designing new molecular systems for chemical selectivity
  - Establish underlying principles that control the design and control of selectivity at the molecular scale. Develop first-principles, predictive models to design high-affinity ligand molecules and to understand and predict extraction processes.
  - Characterize and understand reaction and separations chemistry to account for the influence of high-dose-rate and high-dose ionizing radiation environments. Explore alternate solvents, such as ionic liquids and supercritical fluids, to yield improved selectivity and separations factors.



Hierarchical synthesis of nanostructured sorbents with enhanced mass transport, increased selectivities and multiple functionalities.



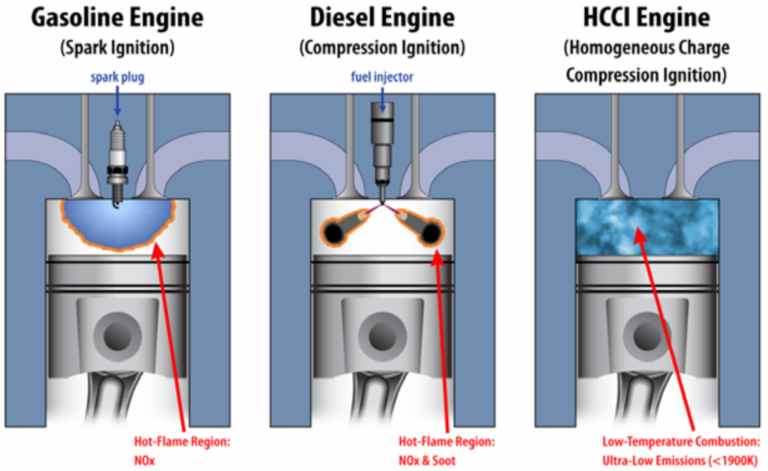
High resolution transmission electron microscopy image of an interface in Cu-Nb nanolayered composite following irradiation with 150 keV He ions to 7 dpa. There is no sign of damage despite significant disruption of the interface by displacement cascades, as shown in the molecular dynamics simulation.

Combustion of Transportation Fuels

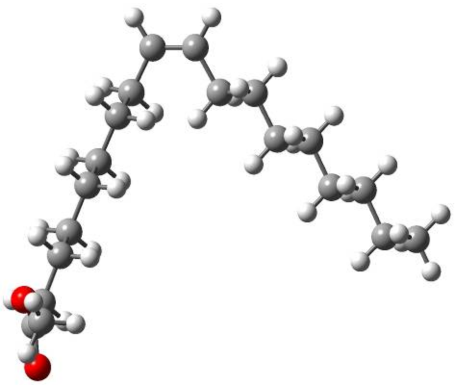
Science Transforming Energy Technologies

Imagine:
- Fully predictive combustion models for the design of new internal combustion engines
- “Smart” engines that adapt in real time to a broad range of new fuels

- Roughly 1/3 of energy use in the U.S. is devoted to transportation and petroleum provides 97% of the energy for the transportation sector.
- Modern IC engine concepts, including homogeneous charge compression ignition (HCCI) and direct injection (DI), are remarkably clean and efficient because combustion is leaner and at a lower temperature.
- Modest enhancements in engine fuel efficiency have major impacts on optimal energy use for transportation in the U.S.
- Fuel streams are evolving rapidly to include fuels from heavy hydrocarbons (oil sands, oil shales, coal) and biofuels (ethanol, other alcohols, biodiesel).
- The challenge: Lean, low-temperature engine technologies are particularly sensitive to variations in the physical and chemical characteristics of fuel. How can fundamental science be brought to bear to optimize the use of non-traditional fuels in cleaner, more efficient engines?



Current and future internal combustion engine concepts

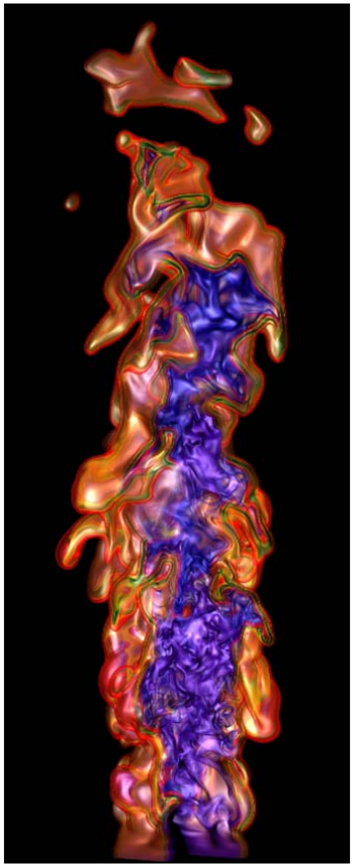


Molecular structure of a methyl ester typically found in soy biodiesel

Basic Research Needs for the Clean and Efficient Combustion of 21st Century Transportation Fuels

Combustion is a complex process, involving hundreds of chemical reactions and coupling of chemistry and turbulent flow. Basic research in chemistry, combustion diagnostics, and combustion simulation are needed to enable the use of 21st century transportation fuels in a manner that optimizes engine efficiency and cleanliness.

- **Predictive modeling of combustion in an evolving fuel environment**
  Predictive modeling is the key to combustion optimization in a non-linear parameter space spanning nine orders of magnitude in space and time. Advances are needed in chemical mechanism development, turbulence-chemistry interactions, algorithm development, and analysis of large data sets.
- **Combustion under extreme pressure**
  Modern engines operate at much higher pressures, demanding fundamental studies of chemical kinetics at high pressure and new theoretical approaches under conditions where the time scales for chemistry and fluid mechanics can no longer be separated.
- **Automated discovery of fuel chemistry**
  New fuels contain larger, more complex molecules whose chemistry is not well known. Automated systems for chemical mechanisms, reaction rates, mechanism reduction, and mechanism validation are required.
- **Spray dynamics and chemistry of new fuels**
  Fuel spray behavior is poorly understood and promises to become more complex with new fuels. Advances are needed multi-phase imaging of sprays and first-principles models for spray breakup.
- **Smart engines**
  An engine that can sense changing fuel streams and dynamically alter its configuration for optimum performance. Real-time analytical and chemical separation techniques must be developed
- **Surface chemistry in combustion**
  Soot modeling needs to be developed to span large spatial and temporal scales. Experimental methods to characterize particle size, shape, chemical composition, and particle precursors are required. Techniques for measuring surface chemistry at high temperature and pressure are needed.



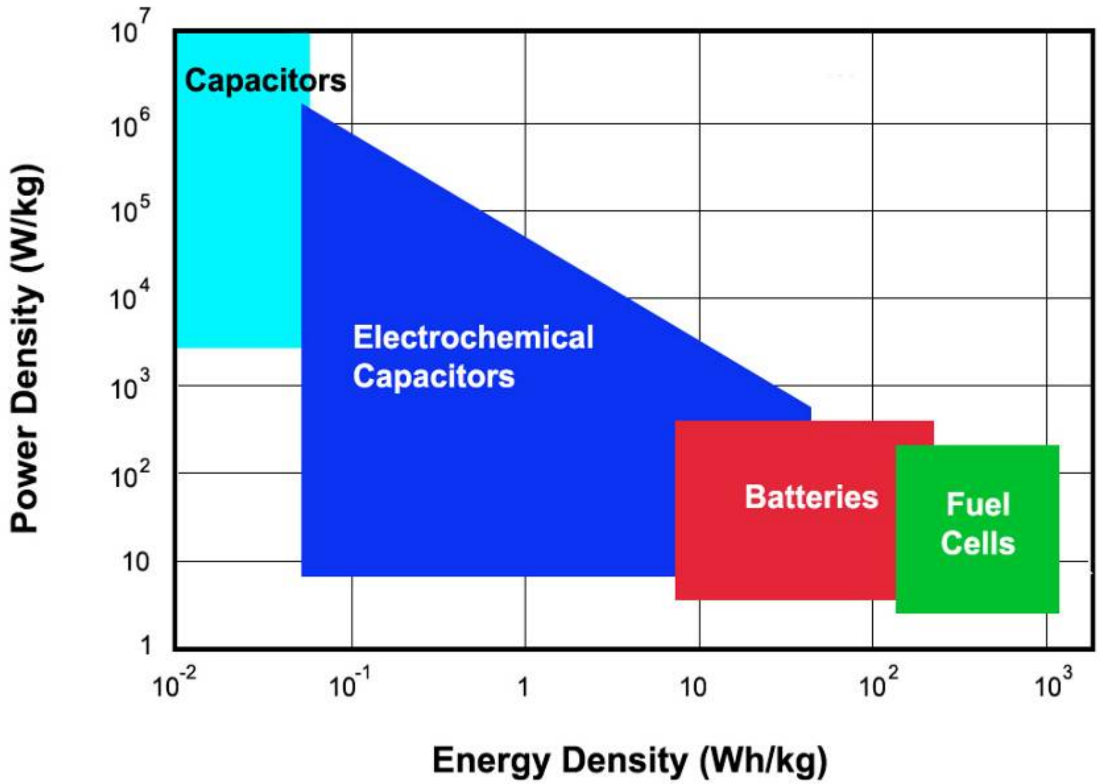
Direct numerical simulation of a turbulent methane-air flame, flowing from bottom to top

Electrical Energy Storage

Science Transforming Energy Technologies

Imagine:
- Solar and wind providing over 30% of electricity consumed in the U.S.
- Numbers of all-electric/plug-in hybrid vehicles exceeding gasoline-powered vehicles

- Many renewable energy sources such as wind and solar are *intermittent*. To make these energy sources truly effective and integrate them into the electrical grid, we need significant breakthroughs in electrical energy *storage* technologies.
- Electrical energy storage (EES) devices with substantially higher energy and power densities and faster recharge times are needed if all-electric/plug-in hybrid vehicles are to be deployed broadly.
- EES devices:
  - Batteries store energy in chemical reactants capable of generating charge
  - Electrochemical capacitors store energy directly as charge.
- Fundamental gaps exist in understanding the atomic- and molecular-level processes that govern operation, performance limitations, and failure of these devices.



Energy and power densities of various energy storage devices. Electrochemical capacitors bridge between batteries and conventional capacitors.

U.S. Department of Energy

Office of Science

Basic Research Needs for Electrical Energy Storage

Basic research in chemical and materials sciences is needed to surmount the significant challenges of electrical energy storage devices for transportation use and to take advantage of large but transient energy sources such as solar and wind.

- **Nanostructured electrodes with tailored architectures**

  Fundamental studies of the electronic conductivity of $LiFePO_4$ led to the discovery of doping-induced conductivity increases of eight orders of magnitude. This research discovery led to the development of high power-density Li-ion batteries by A123 Systems to power electric vehicles such as the Chevy Volt and the Th!nk.

- **The promise of higher battery power via conversion reactions**

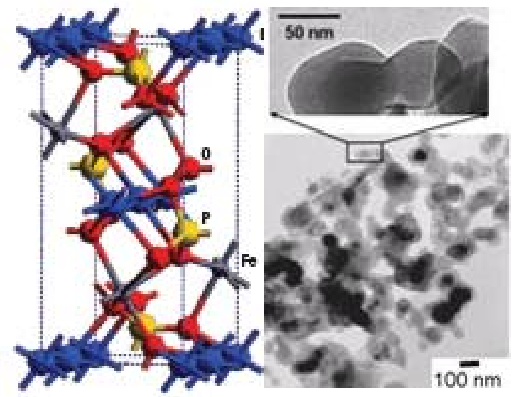
  Current batteries operate with slightly less than one electron per redox center with typical electrode materials. New research on conversion reactions is looking at advanced materials to yield up to six electrons per redox center, allowing a large increase in battery power density. An example of such a reaction using cobalt is: $CoO + 2\,e^{-} + 2\,Li^{+} \leftrightarrows CoO + Li_2O$. Other reactions using sulfides, phosphides and flourides are being investigated.

- **Multifunctional material architectures for ultracapacitors:**

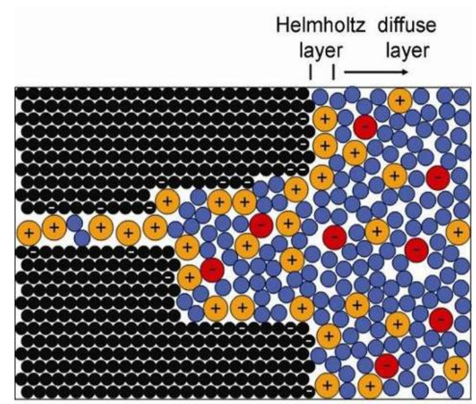
  Basic research in materials for capacitors is enabling the development of multi-functional nanoporous structures and facilitating the understanding of charge storage mechanisms at surfaces. Ultracapacitors complement battery power by allowing very rapid charge and discharge cycles and the high surface area of nanostructures yields high charge storage capacity.

- **Understanding behavior in confined spaces**

  The behavior of electrolytes as a function of pore size in electric double layer capacitors is not well understood but crucial to enabling higher charge densities. Nanometer-scale pores offer high surface areas but create an increased importance of the Helmholz layer in the overall capacitance and affect the dynamics of the charge cycle.



$LiFePO_4$ structural model and nanostructure



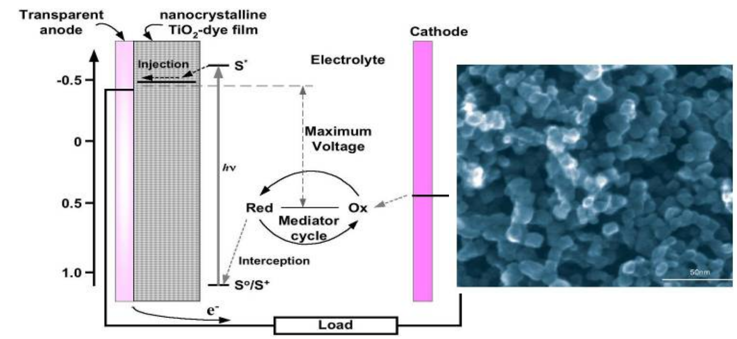
Ion solvation changes with pore size during electric double layer charging (electrode, black; solvent, blue; cation, orange; anion, red)

Hydrogen Economy

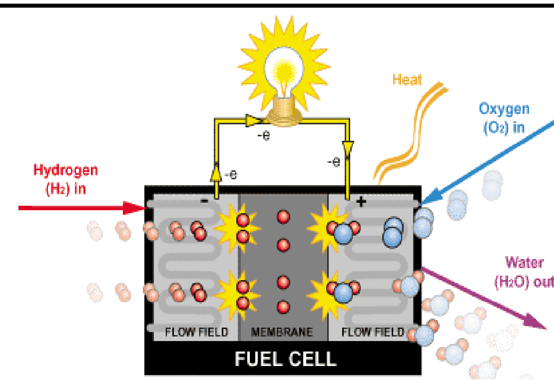
Science Transforming Energy Technologies

Imagine: ▪ A hydrogen economy that provides ample and sustainable energy, flexible interchange with existing energy technologies, and a diversity of end uses to produce electricity through fuel cells.

- The hydrogen economy is a compelling vision, as it provides an abundant, clean, secure and flexible energy carrier. However, it does not operate as an integrated network, and it is not yet competitive with the fossil fuel economy in cost, performance, or reliability.
- There have been significant accomplishments in basic and applied hydrogen research in the past years leading to major advances in hydrogen production, storage, and fuel cell technologies.
- Specifically, hydrogen production from natural gas has met its 2010 target of $3/gge (gallon of gasoline equivalent); hydrogen storage capacities have been increased by 50%; and fuel cells costs have been decreased by 60%.
- But fundamental science breakthroughs are needed in order to meet the longer-term (2015 and beyond) technological readiness requirements.



Dye-Sensitized photoelectrochemical cells for solar hydrogen production via water electrolysis. The cell consists of a highly porous thin layer of titanium dioxide nanocrystal aggregates.

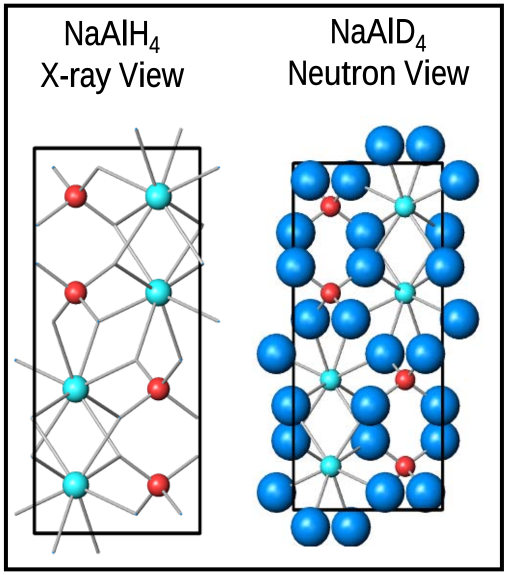


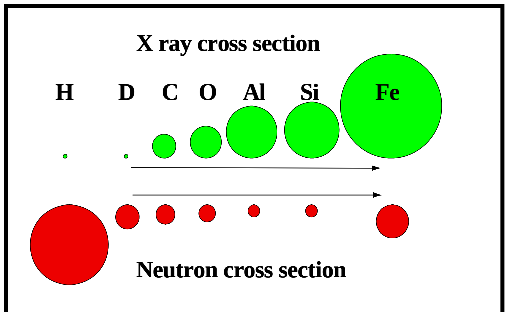
$2H_2 + O_2 \rightarrow 2H_2O$ + electrical power + heat

Basic Research Needs for Hydrogen Production, Storage and Use

The hydrogen economy offers a vision for energy management in the future. Research needs are quintessentially *nano*: catalysis, hydrogen storage materials, and electrode assemblies for fuel cells all depend on nanoscale processes and architecture to achieve high performance.

- Hydrogen Production
  - Fossil Fuel Reforming: Catalytic mechanisms and design, high temperature gas separation
  - Solar Photoelectrochemistry/Photocatalysis: Light harvesting, charge transport, chemical assemblies, bandgap engineering, interfacial chemistry, catalysis, organic semiconductors, theory and modeling
  - Bio- and Bio-inspired H_2 Production: Microbes & component redox enzymes, nanostructured 2D & 3D hydrogen/oxygen catalysis, sensing, energy transduction, biological and biomimetic H_2 production systems
  - Nuclear and Solar Thermal Hydrogen: Thermodynamic data and modeling for thermochemical cycle (TC), high temperature materials: membranes, TC heat exchanger materials, gas separation, improved catalysts
- Hydrogen Storage
  - Metal Hydrides and Complex Hydrides: Degradation, thermophysical properties, effects of surfaces, processing, dopants, and catalysts in improving kinetics, nanostructured composites
  - Nanoscale/Novel Materials: Finite size, shape, and curvature effects on electronic states, thermodynamics, and bonding, heterogeneous compositions and structures, catalyzed dissociation and interior storage phase
  - Theory and Modeling: Model systems for benchmarking against calculations at all length scales, integrating disparate time & length scales, first principles methods applicable to condensed phases
- Fuel Cells
  - Electrocatalysts and Membranes: Oxygen reduction cathodes, minimize rare metal usage in cathodes and anodes, synthesis and processing of designed triple percolation electrodes
  - Low Temperature Fuel Cells: 'Higher' temperature proton conducting membranes, degradation mechanisms, functionalizing materials with tailored nano-structures
  - Solid Oxide Fuel Cells: Theory, modeling and simulation, validated by experiment, for electrochemical materials and processes, new materials-all components, novel synthesis routes for optimized architectures, advanced in-situ analytical tools





Neutron Imaging of Hydrogen

U.S. Department of Energy

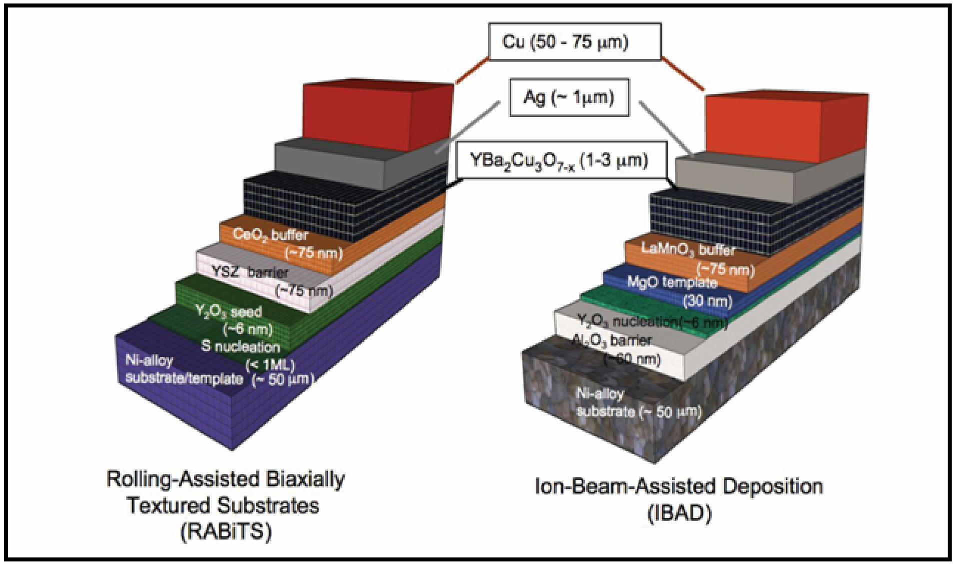
Office of Science

Superconductivity

Science Transforming Energy Technologies

Imagine:
- Smart, resistance-less, and self-healing superconducting electric transmission providing abundant, reliable electricity for the demands of the 21st century.

- Electricity is our most effective energy carrier, providing clean, versatile, switchable power anywhere.
- Current power grid cannot meet the 21st century challenges in capacity, reliability, quality, efficiency.
- Superconductivity offers powerful new opportunities for restoring the reliability of the power grid and increasing its capacity and efficiency.
- Superconductors are capable of carrying current without loss, making the parts of the grid more efficient.
- Unlike traditional grid technology, superconducting fault current limiters can respond to abrupt overcurrents, thus protecting the grid from damage.
- Superconducting motors and generators cut losses, weight, and volume by a factor of two; they are also much more tolerant to voltage variations, frequency instabilities, and reactive power fluctuations than their conventional counterparts.



Schematics of the epitaxial multilayer heterostructures that make up 2nd generation "coated conductors." RABiTS and IBAD are the two approaches being pursued by U.S. industry to yield the near-single crystal YBCO coating needed for high current performance.

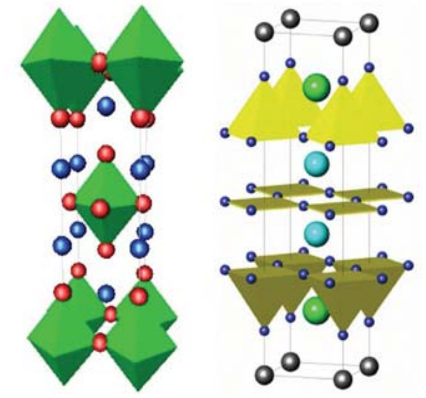
U.S. Department of Energy

Office of Science

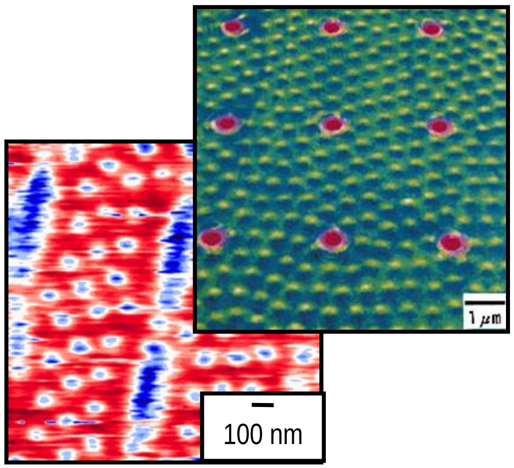
Basic Research Needs for Superconductivity

The challenge of superconductivity is finding the mechanisms of pairing and correlated electron states of high temperature superconductivity. Two decades after their discovery, high-temperature superconductors are viewed less as a singular mystery and more as a threshold to new realms of physics.

- **Develop a comprehensive theory of superconductivity and superconductors**
  Understanding the pairing of electrons and their coalescence into a state of matter that conducts electricity without loss is the conceptual underpinning of superconducting technology and, also, fundamental to materials physics.
- **Understand and exploit competing electronic phases**
  The superconductivity phase is just one of several competing electronic phases (e.g., magnetically ordered or electrically insulating phases) that can be used as new “knobs” to “tune” the performance of superconductors. However, the underlying principles that govern the interplay between these competing phases are unknown.
- **Control structure and properties of superconductors at the atomic scale**
  The growth of highly perfect crystals of many representative compounds in bulk and film form is vital to the understanding of superconductivity in existing complex, strongly correlated materials. Understanding and attaining the performance limits of these materials will require exquisite control through advanced synthesis in order to make them either very pure or controllably defective on many length scales, down to the atomic.
- **Advance the science of vortex matter**
  Recent advances in nanotechnology and in computational as well as experimental techniques provide new opportunities to design and evaluate novel vortex phases and conductor structures that extend the limits of vortex pinning and current-carrying capability to higher temperatures and magnetic fields.
- **Maximize current-carrying ability of superconductors**
  Understanding and controlling the growth mechanisms to produce single-crystal-quality film of complex materials over kilometers of practical conductors challenge our scientific understanding and push our ability to synthesize materials in practical form.
- **Develop the tools to probe electronic matter and vortex matter in real time**
  Higher energy, spatial, and temporal resolution to determine the electronic and magnetic characteristics of the superconducting state.



Crystal structure of the first high-Tc superconductor, $La_{2-x}Sr_xCuO_4$ (left), with a Tc of ~40 K, versus the record holder, $Hg_{0.2}Tl_{0.8}Ca_2Ba_2Cu_3O_8$, with a Tc of ~140 K (right). Because the Cu-O planes are the same in both materials, the huge 100 K difference must result from the optimization of energy scales in the Hg-based compound.



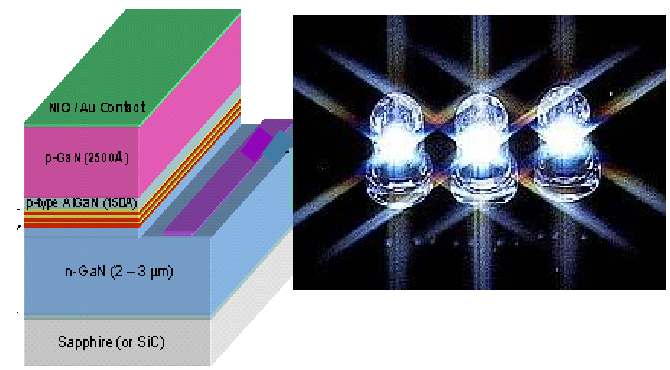
Lorenz electron microscopy (top) and scanning tunneling microscopy images of vortices.

Solid State Lighting

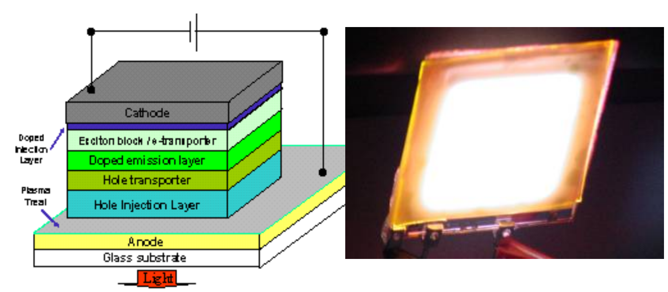
Science Transforming Energy Technologies

Imagine:
- Solid-state lighting producing visible white light with near 100% efficiency
- A solid-state lighting network that is simultaneously high efficiency, low cost, with superior color-rendering quality and long life, and is fully integrated with a smart grid powered by renewable energy sources, such as solar photovoltaics.

- 22% of the nation's electricity (8% of the nation’s total energy) is used for artificial lighting, with a cost of ~$50 billion per year.
- The environmental impact of the lighting energy usage is about 130 million tons of carbon emitted into the atmosphere, or about 7% of all the U.S. carbon emission.
- Current artificial lighting technology, such as incandescent or florescent lighting, are inefficient, with conversion efficiencies in the range of 2 to 20%.
- Solid-state lighting uses the conversion of electricity to visible white light in solid-state materials. By taking advantage of direct electricity-to-light conversion rather than processes in which light is the by-product of another conversion, as with traditional incandescent and florescent lighting, it promises near-100% conversion efficiency.
- An increase in conversion efficiency to 50% will reduce energy consumption in the U.S. by ~620 billion KW-h per year by 2025.



Schematic and image of solid-state lighting based on inorganic semiconducting light emitting diodes (LEDs), which provide point light sources.

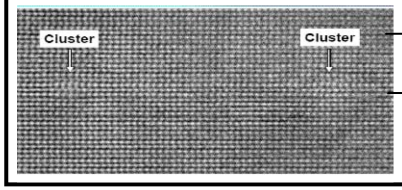


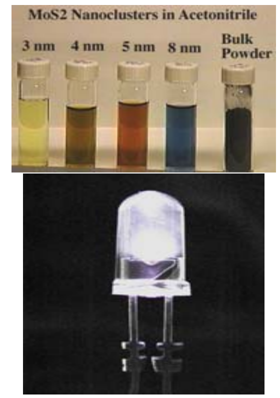
Schematic and image of small molecules-based organic light emitting diodes (OLEDs), which provide diffuse planar light.

Basic Research Needs for Solid-State Lighting

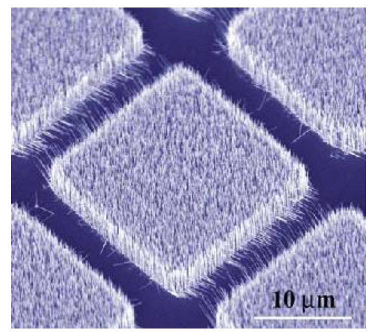
- **New functionality through heterogeneous nanostructures**
  Control of functionality at the nanoscale may enable increased efficiency and enhanced color quality of light sources. Research involves synthesis and assembly; structuring materials to control of radiative and nonradiative processes; and integration into solid-state lighting structures.
- **Innovative photon management**
  Fundamental innovations are required to explore basic photon states and modal properties that enhance spontaneous emission, thermal emission, and light extraction.
- **Enhanced light-matter interactions**
  Identify material and device configurations that enable the strong coupling in a nanocomposite-optical microcavity system; nanoplasmonic enhancement; new electromagnetic pathways for enhanced emission; directed energy transfer pathways; coherent/collective processes; and semiconductor hybrid nanostructures.
- **Multiscale modeling for solid-state lighting**
  Predictive models that reliably describe heterogeneous optoelectronic materials an dlighting devices is critical to solid-state lighting. Research involves adaptive quantum design by harnessing a combination of modern computational power, adaptive algorithms, and realistic physical models; and a hierarchy of models that link the quantum nanoscale, quantum mesoscale, semiclassical mesoscale, and device level models to provide the complete modeling toolkit for solid-state lighting.
- **Precision nanoscale characterization**
  A new generation of characterization tools is needed to provide unprecedented degree of insights for the goal of atom-by-atom design of light emitting materials. Research involves near-field optical microcopy to reach beyond the diffraction limit; single molecule spectroscopy to determine properties of individual molecules; electron microscopy and microspectroscopy towards sub-Å resolution; x-ray scattering and spectroscopy; and tools for organic assay for achieving high purity materials.

Nanoscale Indium clustering in InGaN
LBNL and Lumileds CRADA, NCEM HRTEM image





Nanoscale phosphors for white light LED emission.

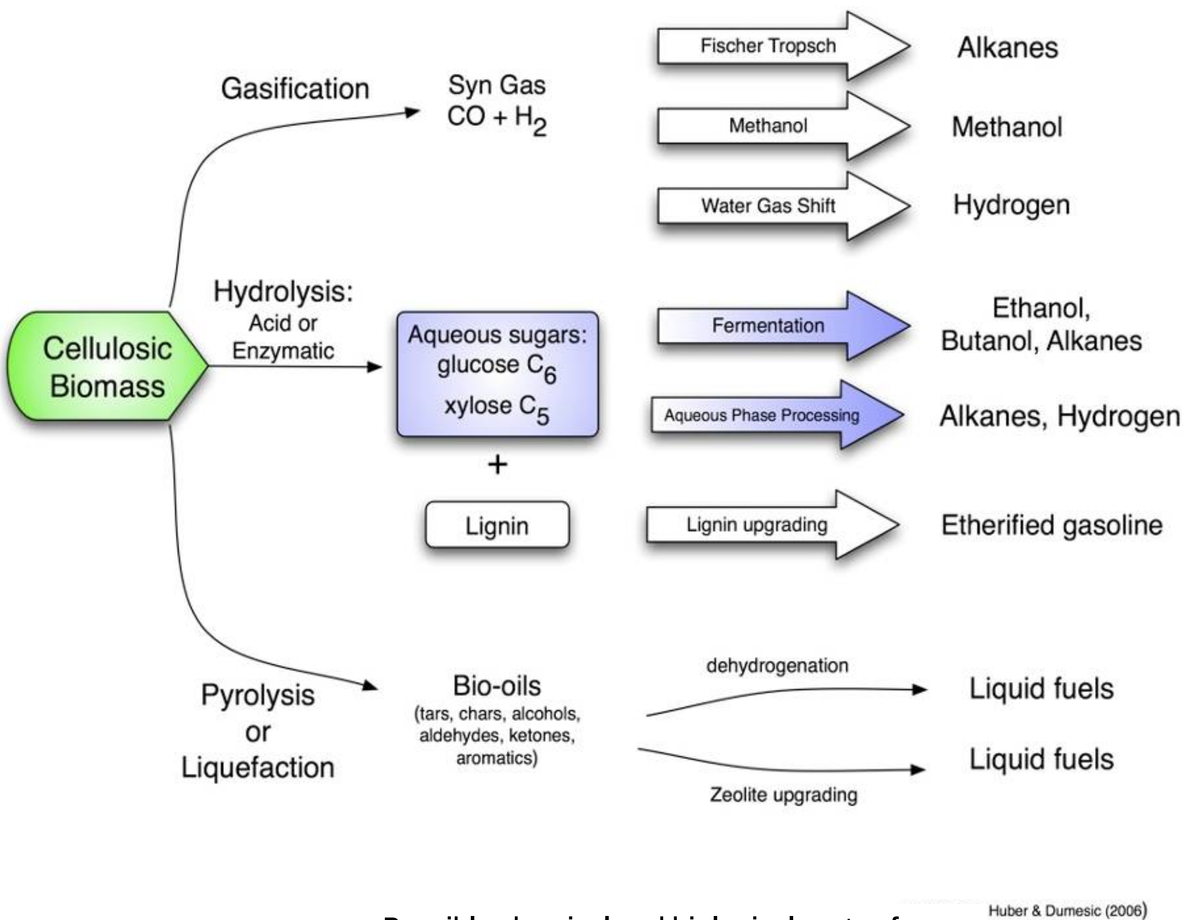


Patterned GaN nanowire arrays grown via metal organic chemical vapor deposition, showing precision control of nanostructure synthesis.

Catalysis
Science Transforming Energy Technologies

Imagine:
- Catalytic processes for turning biomass into hydrocarbon fuels, not ethanol
- Robust methods for “refining” non-traditional fossil feedstocks into liquid fuels

- Catalysis is essential to the current production of fuels and chemicals from petroleum. But current catalytic processes used in refining petroleum cannot be used for new, more complex feedstocks.
- New classes of catalysts are required for the conversion of future feedstocks to fuels:
  - Heavy fossil (shale oil, tar sands, coal) – variations in physical and chemical composition of these feedstocks demand new catalytic processes
  - Renewables (biomass) – how can cellulose and lignin be deconstructed chemically? Can reactions be developed to remove oxygen and increase H/C ratios?
  - Carbon dioxide and water – can efficient photo- or electrocatalytic methods be developed to turn these abundant feedstocks into fuels?



Possible chemical and biological routes from celluosic biomass to liquid fuels

U.S. Department of Energy

Office of Science

Basic Research Needs: Catalysis for Energy

Meeting the demands for new catalysts for energy requires a fundamental understanding of the mechanisms and dynamics of catalyzed reactions that will allow the design and synthesis of new catalytic structures at the atomic and nano scale.

- Grand challenges for catalysis science

  Understanding the mechanisms and dynamics of catalyzed reactions at the atomic and molecular scale. Requires new tools to image surfaces at the atomic scale and to probe the structures and energetics of the reacting molecules on multiple time and length scales. Theory must be developed to validate the results. The influence of the environment on the function of the catalyst must be better understood

  Design and controlled synthesis of catalyst structures. Interplay between characterizing catalysts as they function and synthesis of new catalysts to achieve high activity and product selectivity. Predictive theory is required.

- Advanced catalysts for the conversion of heavy fossil energy feedstocks

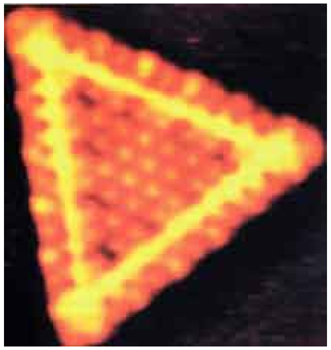
  The wide variation in chemical composition demands improved chemical analysis of feedstocks. The dependence of catalyst function on its environment must be elucidated. Better catalysts are needed for heteroatom removal, better selectivity, and use of alkanes as co-reactants.

- Advanced catalysts for the conversion of biologically derived feedstocks

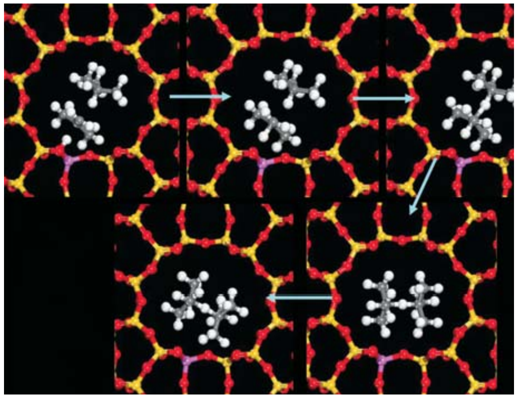
  Understand the catalytic deconstruction of cellulose and lignin at the molecular level. Design and understand reactions that remove oxygen and increase the hydrogen-carbon ratio. Find whole new classes of catalysts for both of these types of conversions.

- Advanced catalysts for the photo- and electro-driven conversion of carbon dioxide and water

  Understand in detail how multi-electron transfer reactions, such as photosynthesis, occur. Improve the coupling of the input (radiation or electrons) with the chemical conversion. Establish a foundation for the prediction of multifunctional catalysts.

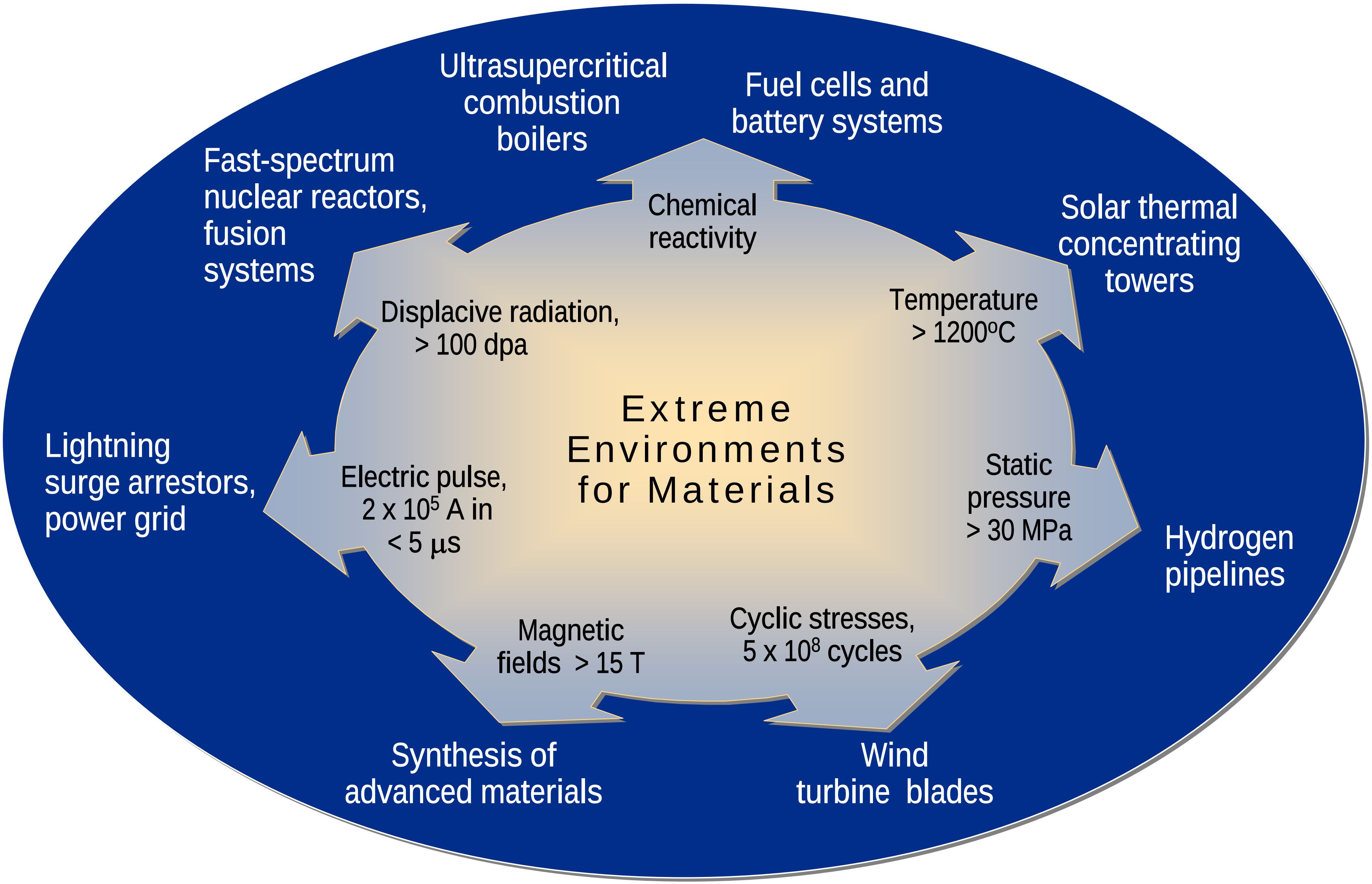


TEM image of a model molbydenum disulfide catalyst showing layers that are only a few atoms across



Computed mechanism for the catalytic coupling of two four-carbon molecules to create an eight-carbon, fuel-like molecule

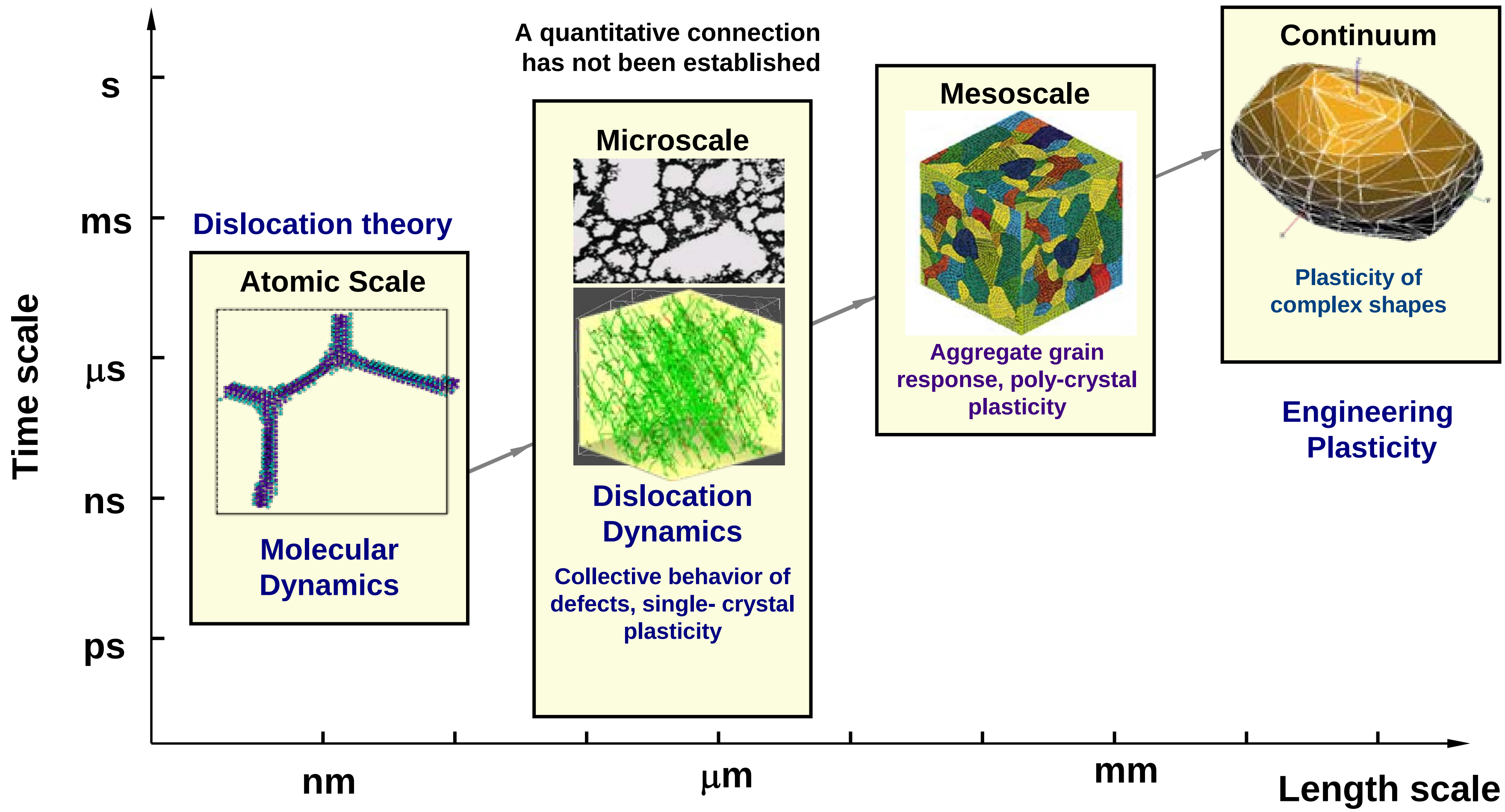
Extreme Environments in Energy Applications



U.S. Department of Energy

Office of Science

Multi-scale Simulation: the Cross-Cutting Challenge



Today: Manually connect the length and time scales

Tomorrow: Self-assembled algorithms automatically adjust length and time scales

U.S. Department of Energy

Office of Science

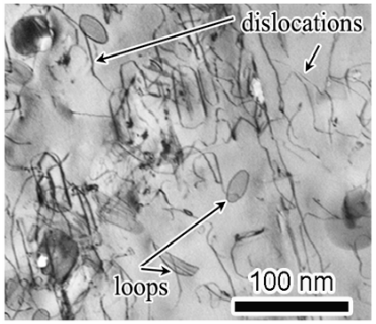
Materials under Extreme Environments

Science Transforming Energy Technologies

Imagine:
- Reaching the fundamental limit of materials performance
- Designing radically new materials by exploiting extreme conditions

- Materials are central to every energy technology; future energy technologies will place increasing demands on materials performance.
- The extreme environments in energy applications include stress, strain, temperature, pressure, chemical reactivity, photon or radiation flux, and electric or magnetic fields.
- Future energy technologies will put increasing demands on materials performance. These increasingly extreme operating environments accelerate the aging process in materials, leading to reduced performance and eventually to failure.
- Materials failure is the principal bottleneck for developing future energy technologies. Fundamental gaps exist in understanding the atomic- and molecular-level processes that govern operation, performance limitations, and failure of materials operated under extreme environments in energy applications.

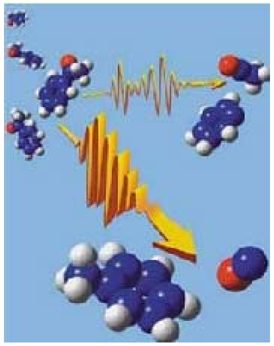
Neutron Damage on Stainless Steel

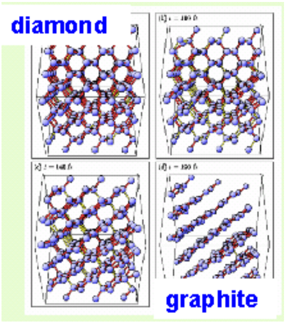


Displacement cascades grow to microstructural defects .

Control 1.5 x 10^{23} n cm^{-2}

20% CW 316 stainless steel, 796 K



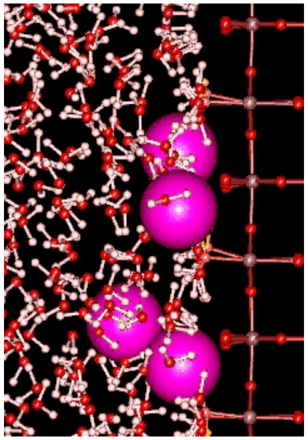


Manipulating matter with photons provides pathway to induce phase transitions, e.g., from diamond to graphite, as shown by atomistic simulation.

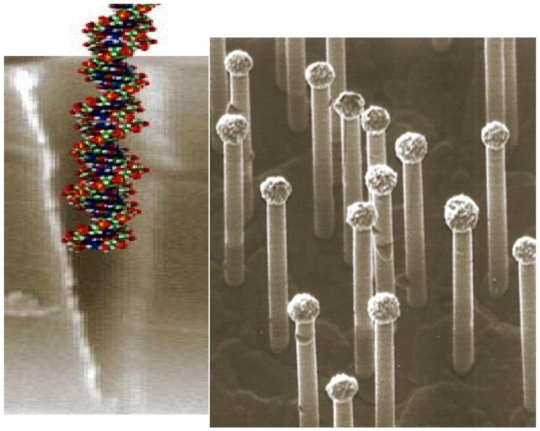
Basic Research Needs for Materials under Extreme Environments

Reaching the intrinsic limit of materials performance requires understanding the atomic and molecular origins of materials failure. This will enable discovery of new materials by exploring atomic and molecular manipulation at the extremes.

- **Design of materials with revolutionary tolerance to extreme photon and particle fluxes**
  Understanding the origins of performance limits of materials under high flux environments over the full range of time and length scales; developing defect-free, defect-tolerant, or self-repairing materials for application in high flux environments.
- **Toward ideal surface stability**
  Coupled experimental and theoretical developments and modeling to allow predictive capabilities for long-term stability, in particular the role of nanoscale defects throughout the film-substrate system; and correlate the defects with breakdown locations and mechanisms to determine the causes of loss of chemical and mechanical stability.
- **Control and synthesize materials with new properties using photon and particle beams**
  Understanding how energetic particle and photon beams interact with matter and learning how to control and manipulate these interactions to create targeted phases and structures.
- **Controlling reaction dynamics at extremes**
  Obtaining a detailed understanding of the atomic and molecular mechanisms responsible for the reactivity and synthesis of materials under the full range of extreme conditions and the ability to predict the structure of formed phases.
- **High performance electric and magnetic material systems**
  The exploration of correlated electron behavior in extreme electric and magnetic fields and the use of extreme fields to synthesize new materials will enable powerful new directions for the discovery of new materials and phenomena.
- **Exploring thermomechanic limits of materials**
  Obtaining a detailed understanding that defines possible critical dimensions for dislocation generation and multiplication, as well as potential length-scale or architecture effects on elastic strain relationships in composite materials.



Ab initio density functional theory is used to model interfacial solution structure and energetics and to provide interaction potentials for incorporation into large scale simulation.



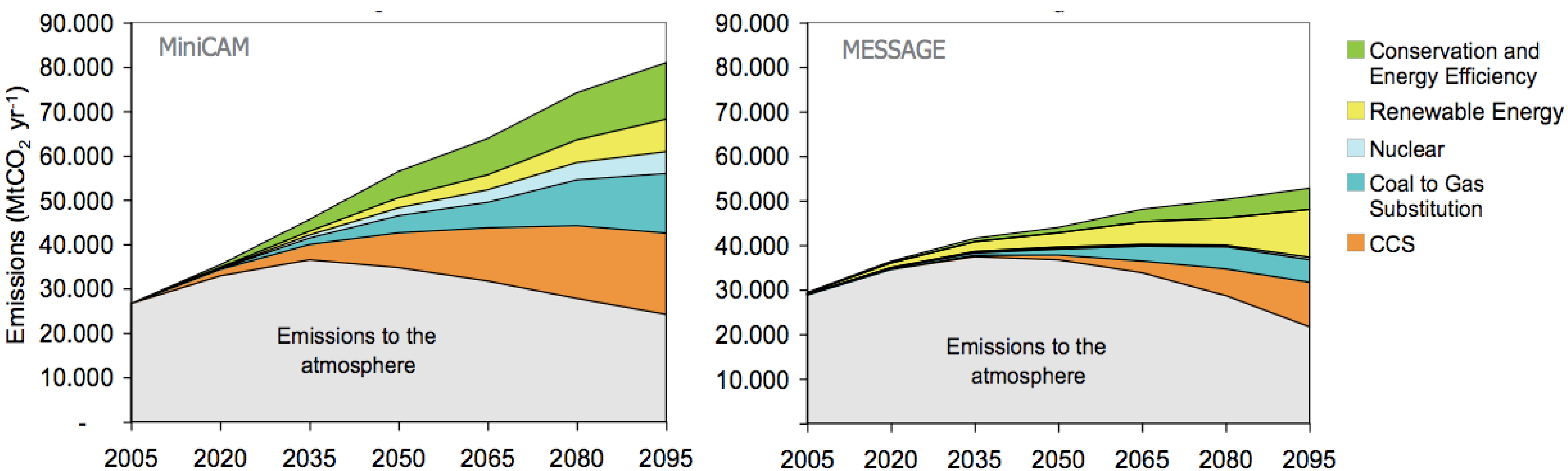
Single Nanopore
Nanowires

Nanopores created by etching track left by heavy ion damage (left) and nanorods formed by filling nanopores and removing the matrix (right).

Geosciences

Science Transforming Energy Technologies

Imagine:
- Safe and environmentally benign underground sequestration of CO_2 for centuries
- Safe and environmentally benign underground storage of spent nuclear fuel for millennia



Two scenarios for reducing carbon dioxide emissions to keep atmospheric concentrations at 450-750 ppmv. Left: high-emission scenario, where nuclear plays an important role. Right low-emission scenario. In both cases, carbon capture and storage (CCS) – the orange wedge - plays a critical role. (IPCC report, 2007)

- Continued use of fossil fuel while capping the atmospheric concentration of carbon dioxide to about double the pre-industrial level requires the sequestration of ~10 GT of CO_2 per year.
- Tenfold expansion of current nuclear technology to reduce carbon emissions requires the storage of spent nuclear fuel at a global rate of ~1 Yucca Mt per year.
- "Underground" as a long-term storage container
  - Advantages: Enormous volume; distance from subsurface environment; pre-made container
  - Disadvantages: Designed by nature, only approximately fits the design criteria for containment; complex materials and processes; difficult to see and monitor; uncertainty about long-term performance (100 – 1 million yrs)

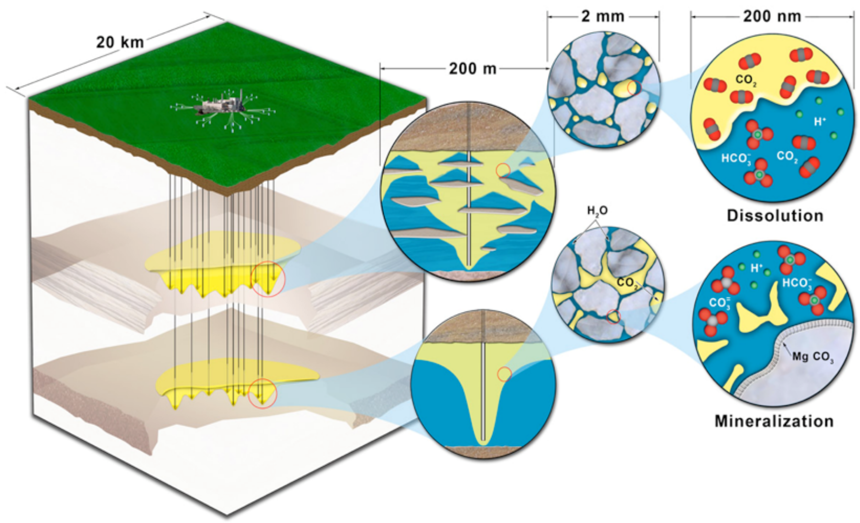
U.S. Department of Energy

Office of Science

Basic Research Needs in Geosciences: Facilitating 21st Century Energy Systems

A science-based approach is required to understand the long-term behavior of subsurface geological systems in which anthropogenic carbon dioxide and nuclear materials can be safely and securely stored for centuries to millennia.

- Grand challenges in geosciences
  - Computational thermodynamics of complex fluids and solids. New models are needed for translating from the atomic and molecular scale to the subsurface scale.
  - Integrated characterization, modeling, and monitoring of geological systems. Current diverse methods for monitoring and modeling need to be linked in a revolutionary and coordinated manner.
  - Simulation of multi-scale geological systems over ultra-long times. Major advances in modeling across spatial and temporal scales required.
- Cross-cutting research issues
  - The microscopic basis of macroscopic complexity. Scale separation is often missing in geological systems, where emergent behavior plays a critical role.
  - Highly reactive subsurface materials and environments. Storage creates compositionally complex systems with rich chemistry, gradients in pressure and temperature, and radiation fields.
  - Thermodynamics of the solute-to-solid continuum. Rigorous structural, kinetic, and thermodynamic descriptions of complex chemistry from the molecular scale to the macroscopic scale is lacking.
- Priority research directions
  - Mineral-water interface complexity and dynamics.
  - Nanoparticulate and colloid physics and chemistry.
  - Dynamic imaging of flow and transport.
  - Transport properties and *in situ* characterization of fluid trapping, isolation, and immobilization.
  - Fluid-induced rock deformation.
  - Biogeochemistry in extreme and perturbed environments.



Storage of carbon dioxide in an underground formation (left) is a highly non-equilibrium system with features at multiple spatial scales. The center insert shows CO2 as a mobile phase (lower) and trapped residual phase (upper) at a scale of 100 meters. The insets at right show nanometer scale mechanisms of CO2 trapping – dissolution (upper) and mineralization (lower).

Energy Frontier Research Centers

Engaging the talents of the nation's researchers for the broad energy agenda

Energy Frontier Research Centers will bring together the skills and talents of multiple investigators to enable research of a scope and complexity that would not be possible with the standard individual-investigator or small-group award.

The DOE Office of Science, Office of Basic Energy Sciences, announced the Energy Frontier Research Centers (EFRCs) program. EFRC awards are $2–5 million/year for an initial 5-year period. Universities, labs, and other institutions are eligible to apply.

Energy Frontier Research Centers will pursue fundamental research that addresses both energy challenges and science grand challenges in areas such as:

- Solar Energy Utilization
- Catalysis for Energy
- Electrical Energy Storage
- Solid State Lighting
- Superconductivity
- Bioenergy and biofuels
- 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

U.S. Department of Energy

Office of Science

A123 Systems *(Yet-Ming Chiang, MIT)*

A123 SYSTEMS

TECHNOLOGY | APPLICATIONS | PRODUCTS | NEWS | COMPANY

power. safety. life.

OVERVIEW | POWER | SAFETY | LIFE

Based on new, highly active nanoscale material initially developed at MIT, A123Systems' low impedance Nanophosphate electrode technology provides significant competitive advantage over alternative high power technologies.

Our cell and electrode designs are optimized for low cost/watt and cost/watt-hour performance. They have higher voltage than other long-life systems, enabling lower pack cost. Their long life leads to reduced lifecycle and system costs resulting in greater overall price-performance.

A123Systems can develop a customized power solution to fit your energy needs, whether your products use rechargeable batteries, disposable batteries, 120V or 220V AC power, compressed air, or internal combustion engines. A123Systems' novel technology offers new performance features that could revolutionize your products. To obtain additional information about our products or investigate our battery products for your application, please contact us or use our product evaluation form.

+ product features

Power

+ Over 100C pulse discharge rates
+ Ultra fast charge
+ Consistent discharge/regen power over wide state-of-charge

Safety

+ Inherently safer chemistry
+ Superior abuse tolerance

Life

+ 10+ year projected calendar life
+ Industry leading cycle life
+ Environmentally friendly chemistry

+ get started

Tell Us About Your Application

Order Your Developer's Kit

LBNL Materials Sciences Spin-Off Companies

Berkeley Lab

- Solexant
- PolyPlus Battery Company
- ATI (Ariel Technologies, Inc.)
- Momenta
- Symyx®
- MMFX Technologies Corp
- SEEO
- Electric Fuel®
- nanomix (nano.com)
- QuantumDot
- Superconductor Technologies — Improving the Quality of Wireless℠

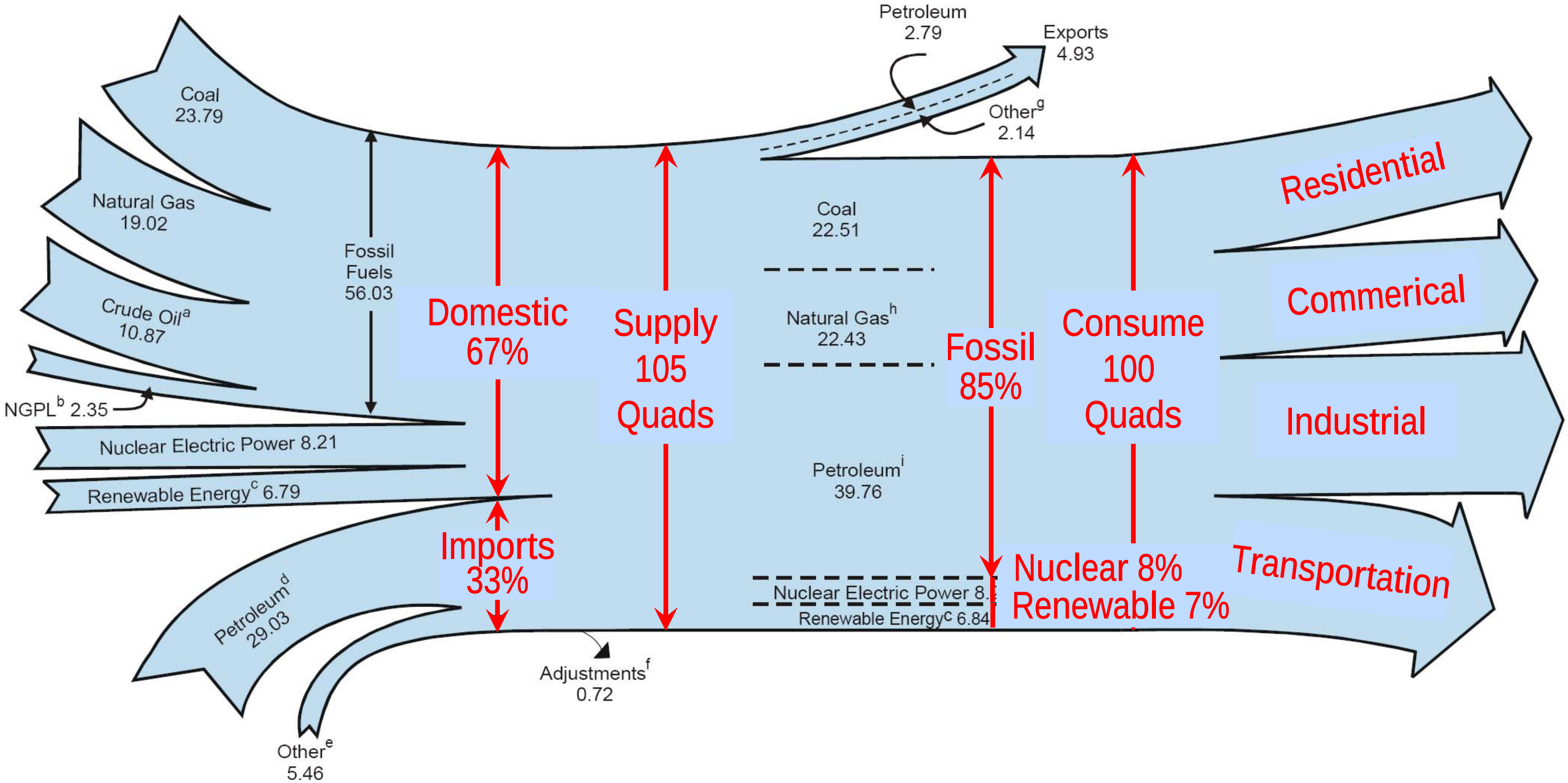
Market Capitalization ~$1.5 Billion

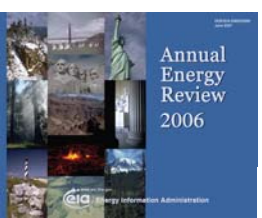
Thank You!

http://www.sc.doe.gov/bes/bes.html

U.S. Energy Flow, 2006 (Quads)

85% of primary energy is from fossil fuels



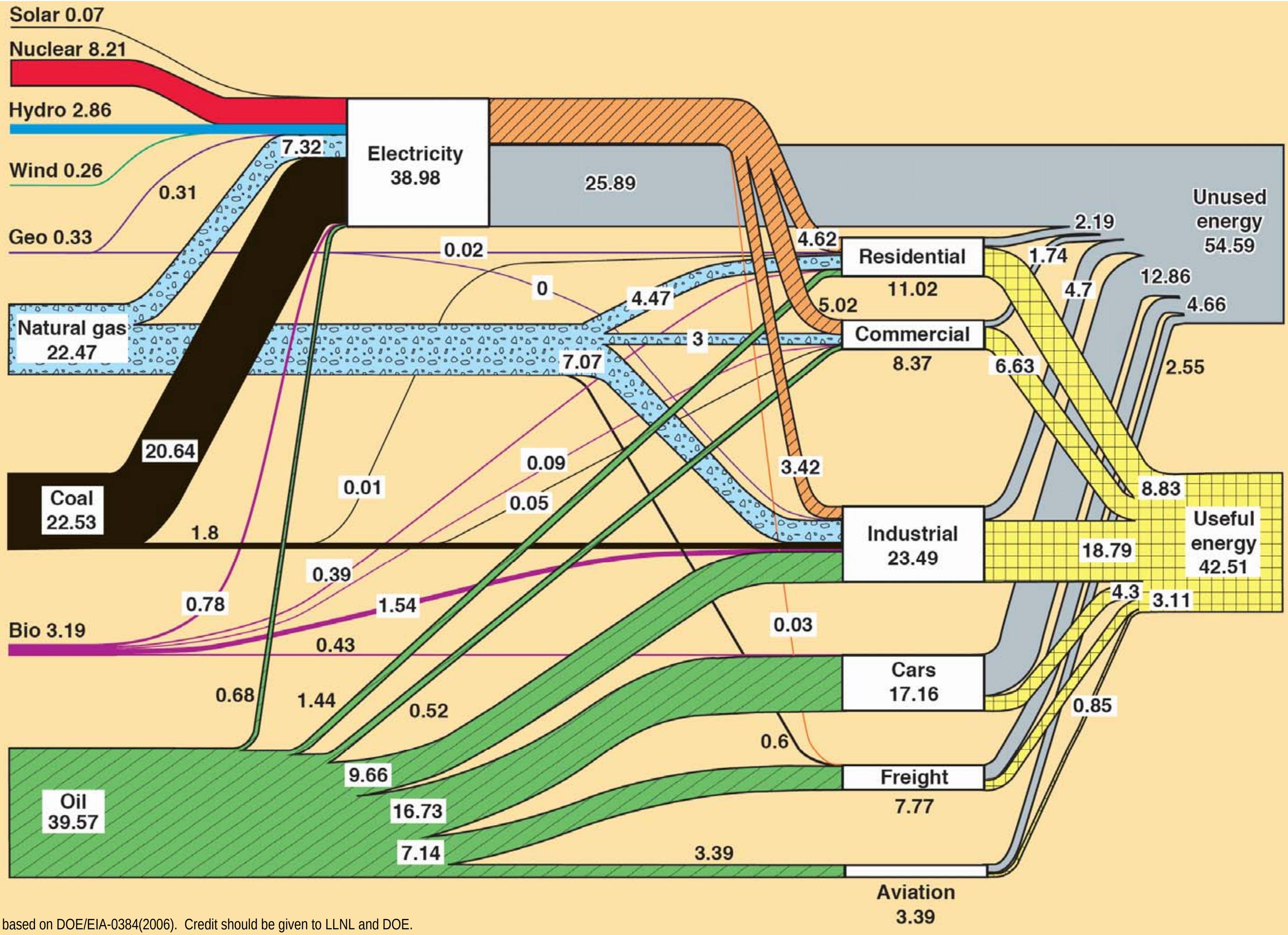


U.S. Department of Energy

Office of Science

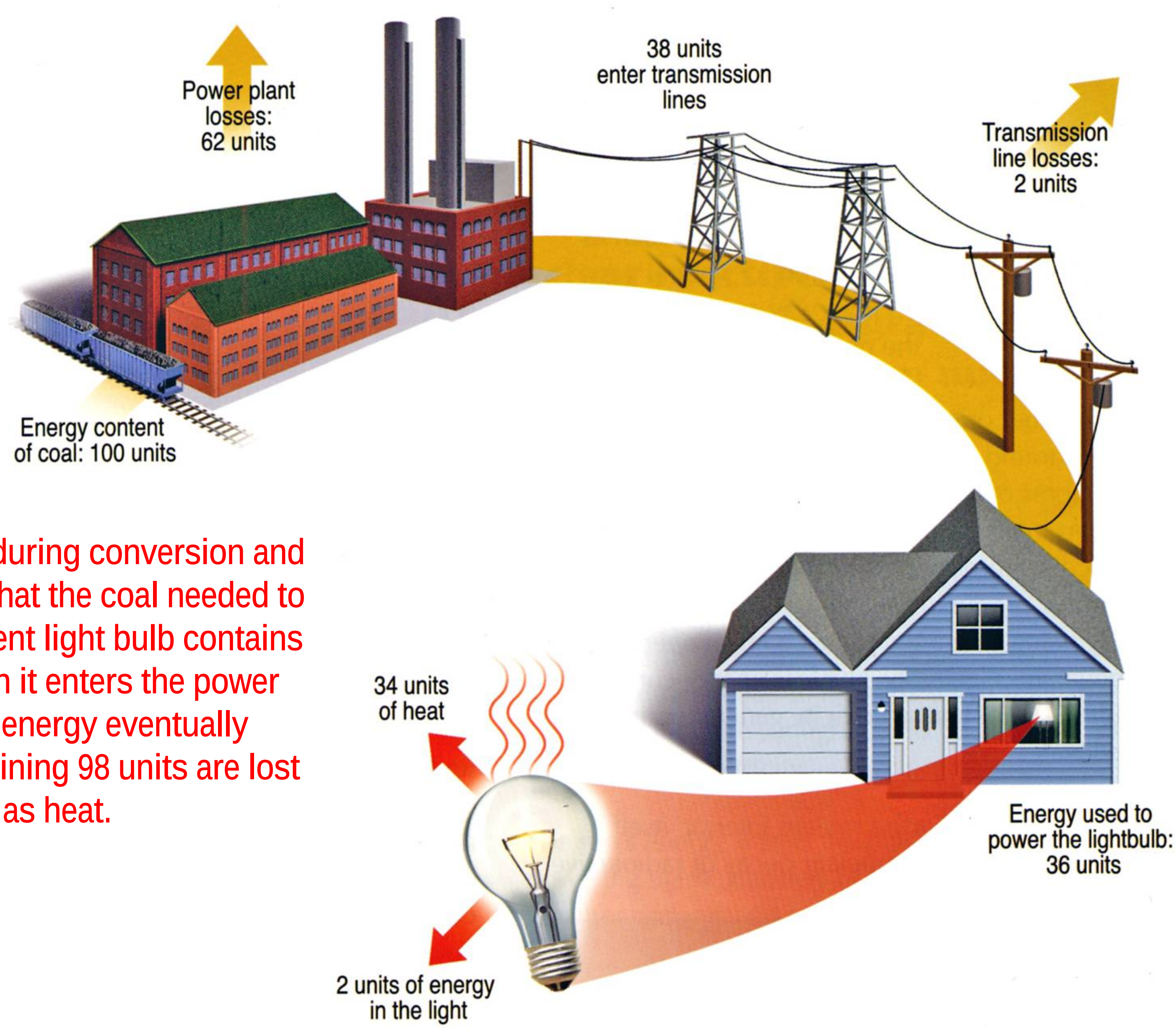
U.S. Energy Flow, 2006 (Quads)

>70% of primary energy for the transportation sector and >60% of primary energy for electricity generation/use is lost



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

Overall Efficiency of an Incandescent Bulb ≅ 2%



Example of energy lost during conversion and transmission. Imagine that the coal needed to illuminate an incandescent light bulb contains 100 units of energy when it enters the power plant. Only two units of energy eventually light the bulb. The remaining 98 units are lost along the way, primarily as heat.