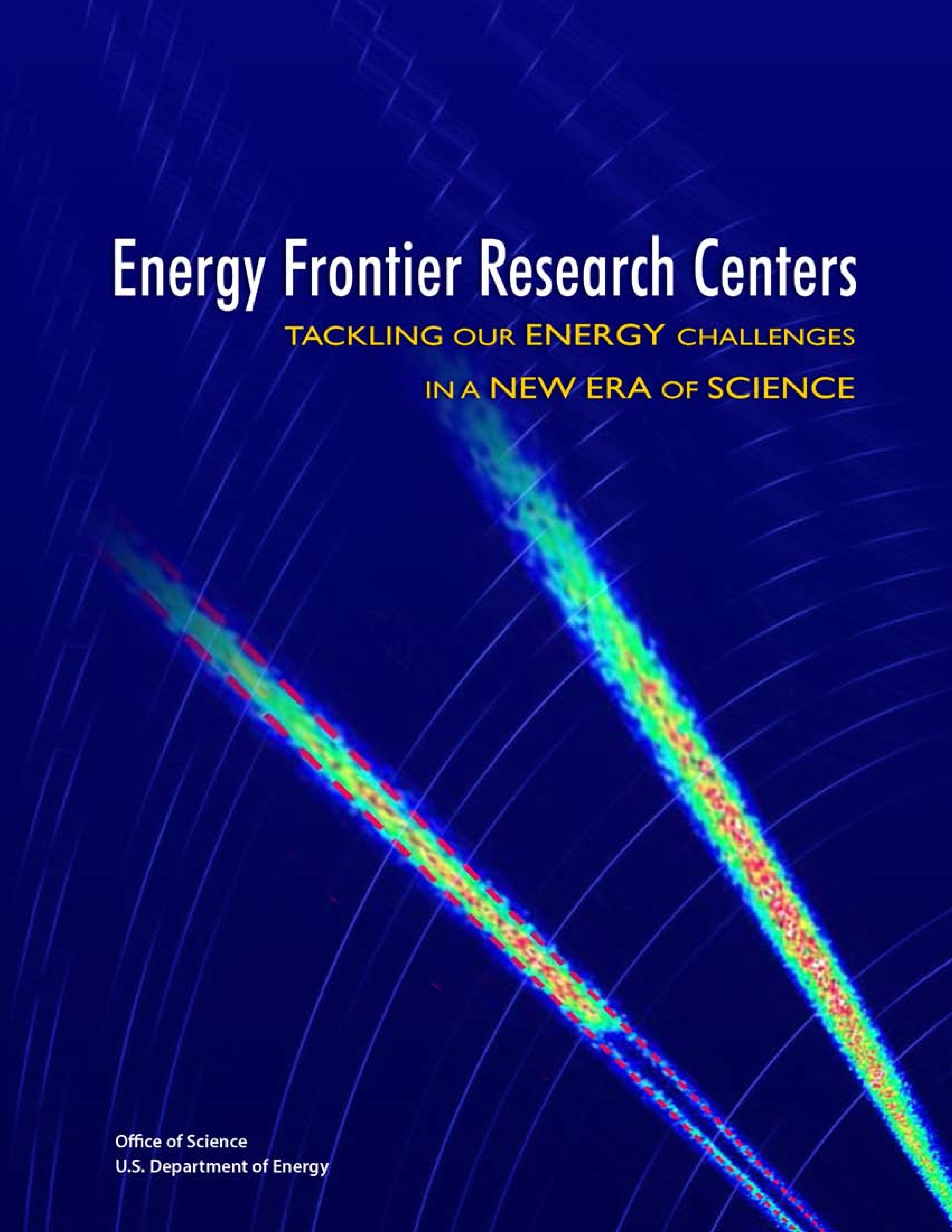


# Energy Frontier Research Centers

## TACKLING OUR ENERGY CHALLENGES IN A NEW ERA OF SCIENCE

Office of Science
U.S. Department of Energy

*On the Cover:*

*Atomic-scale spatial resolution and femtosecond temporal resolution techniques provide new means of visualizing and controlling materials far from equilibrium, enabling the "grand challenge" scientific discovery research required to understand energy relevant materials and processes. Femtosecond x-ray scattering snapshots of materials driven far from equilibrium are shown where time has been transformed into space, thus capturing the ultrafast changes in the x-ray diffracted intensity associated with structural phase transitions in the semiconductor InSb. (From A.M. Lindenberg et al., "Atomic-scale visualization of inertial dynamics,"* Science*,* ***308****, 392 [2005].)*

*Work performed at the Stanford Linear Accelerator Center by the Sub-Picosecond Pulse Source Collaboration, supported, in part, by Basic Energy Sciences, U.S. Department of Energy.*

EFRC ENERGY FRONTIER RESEARCH CENTERS

For further information and updates on the Energy Frontier Research Centers, please visit http://www.sc.doe.gov/bes/EFRC.html.

U.S. DEPARTMENT OF ENERGY

Office of Science U.S. DEPARTMENT OF ENERGY

Office of Basic Energy Sciences • Serving the Present, Shaping the Future •

# Contents

# Introduction

As world demand for energy rapidly expands, the United States finds itself in an intensifying global competition for energy resources. Transforming the way we generate, supply, transmit, store, and use energy will be one of the defining challenges for America and the globe in the 21st century. At its heart, the challenge is a scientific one. Fortunately, American science today is entering on a new era of discovery, equipped with a powerful new generation of tools for penetrating, understanding, and manipulating matter on the atomic and molecular scales. These new capabilities have profound implications for our ability to harvest new sources of energy and to utilize the energy we have with decisively greater efficiency. The key is to mobilize the talents and creativity of our national scientific workforce in a focused nationwide effort to meet our energy challenges.

To do so, the Office of Basic Energy Sciences in the U.S. Department of Energy's Office of Science is establishing a $100 million Energy Frontier Research Centers (EFRCs) initiative. Under this initiative, universities, national laboratories, nonprofit organizations, and for-profit firms will be invited to compete, singly or in partnerships, to establish an EFRC. Centers will be selected by scientific peer review and funded at $2-5 million per year over a 5-year period. These integrated, multi-investigator Centers will conduct fundamental research focusing on one or more of several "grand challenges" recently identified in major strategic planning efforts by the scientific community. The purpose of these Centers will be to integrate the talents and expertise of leading scientists in a setting designed to accelerate research toward meeting our critical energy challenges. The EFRCs will harness the most basic and advanced discovery research in a concerted effort to establish the scientific foundation for a fundamentally new U.S. energy economy. The outcome will decisively enhance U.S. energy security and protect the global environment in the century ahead.

# Background Information

### *Context*

The 21st century brings with it staggering challenges for advanced energy technology. Limited supplies of traditional fossil energy resources and the negative global effects of traditional fossil fuel utilization demand the discovery of transformative energy technologies for the development and effective utilization of new energy sources that are abundant, clean, and economical. Incremental advances in current energy technologies will not address the energy challenges of the 21st century. History has demonstrated that radically new technologies arise from disruptive advances at the science frontiers. The modern marvels of information technology provide the most striking example. Looking to the future: imagine a virtually unlimited supply of electrical power from solar-energy systems, modeled on the photosynthetic processes utilized by green plants, and power lines that could transmit this electricity from the deserts of the southwest to the Eastern Seaboard at nearly 100 percent efficiency. This is but one of many visions of a new energy future that can only come from continuing to push the frontiers of science.

### *Establishing the Energy Research Directions*

The Basic Energy Sciences (BES) program supports fundamental research in focused areas of the natural sciences in order to expand the scientific foundations for new and improved energy technologies and for understanding and mitigating the environmental impacts of energy use. BES has long invested in innovative basic research aimed to achieve this mission through its core research areas. In 2001, the Basic Energy Sciences Advisory Committee (BESAC) conducted a far reaching study to assess the scope of fundamental scientific research that must be considered to address the DOE missions in energy efficiency, renewable energy resources, improved use of fossil fuels, safe and publicly acceptable nuclear energy, future energy sources, and reduced environmental impacts of energy production and use.

The scientific community enthusiastically responded to this BESAC study through participation in a week-long workshop and results were published in early 2003 in the report, *Basic Research Needs to Assure a Secure Energy Future*. That report inspired a series of ten follow-up *Basic Research Needs* workshops over the next five years, which together attracted more than 1,500 participants from universities, industry, and DOE laboratories. Topics included the hydrogen economy, solar energy utilization, superconductivity, solid-state lighting, advanced nuclear energy systems, combustion of 21st century transportation fuels, electrical-energy storage, geosciences as it relates to the storage of energy wastes (the long-term storage of both nuclear waste and carbon dioxide), materials under extreme environments, and catalysis for energy-related processes.

## *The New Era of Science*

Together, these workshop reports highlighted the remarkable scientific journey that took place during the past few decades. The resulting scientific challenges, which no longer were discussed in terms of traditional scientific disciplines, described a new era of science — an era in which materials functionalities would be designed to specifications and chemical transformations would be manipulated at will. Over and over, the recommendations from the workshops described similar themes — that in this new era of science, we would 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, and those skilled in applied mathematics and computer science.

## *The Science Grand Challenges*

This goal to direct and control matter at the quantum, atomic, and molecular levels requires a change in our fundamental understanding of how nature works. A BESAC Grand Challenges subcommittee was convened, which examined the primary roadblocks to progress. The results of that examination were presented in the report, *Directing Matter and Energy*: *Five Challenges for Science and the Imagination*, where a new era for energy science was posed in five challenges. Addressing these grand challenges provides a path forward to the transition from observation to control of matter.

- ***How do we control material processes at the level of electrons?***

  *Much of the last century has focused on understanding how electrons in matter — their charge, their spin, and their dynamics — determine the properties of materials and how they direct chemical, electrical, or physical processes in materials. We are now on the verge of a new science of quantum control where our tools will go beyond probing what is there, towards the goal of controlling these processes and properties through direct manipulation of electrons.*

- ***How do we design and perfect atom- and energy-efficient synthesis of revolutionary new forms of matter with tailored properties?***

  *The periodic table contains more than 110 elements, but only a tiny fraction of all possible chemical compounds has yet been prepared and their properties characterized. In the 21st century, advances in theoretical understanding and computational power and methodology might turn the design rules for materials upside down. At present, we have little understanding of what it will take to achieve this. Beginning with a set of desired materials properties, the specific type of atoms and the arrangement needed to achieve the desired target materials will be defined in a computer. With this as a guideline, the materials designer can set out to bring truly extraordinary materials into a tangible reality.*

**How do remarkable properties of matter emerge from complex correlations of atomic or electronic constituents and how can we control these properties?**

*Uncovering the fundamental rules of correlations and emergence, and achieving control over those correlations, are prospects that can only now be reasonably contemplated with the advent of tools to probe and affect particles and their correlations on the nanoscale. By understanding and controlling correlations, we can put emergence to work for us. The potential applications are as rich as the variety of emergent phenomena.*

**How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things?**

*Implementation and utilization of complex nanotechnologies with capabilities approaching those found within the biological world is quite beyond reach at present. Many functionalities of living systems exceed those of most comparable human engineered technologies by so great a margin that, if it were not for the* a priori *existence of life, they might be inconceivable. But living systems do exist; life thus provides the proof-of-concept for what can physically be achieved with nanotechnology. The ways in which energy, entropy, and information are manipulated within living nanosystems provide us with lessons on what we must learn to do in order to develop similarly sophisticated technologies.*

**How do we characterize and control matter away — especially very far away — from equilibrium?**

*When systems are not at equilibrium, some of the most powerful science that we have, from thermodynamics to statistical mechanics, can become almost useless. This raises practical problems from how efficient a biological motor can be to how stable a glass is. But it also raises a fundamental challenge: how do we characterize and understand matter and information systems away (especially very far away) from equilibrium? These problems arise across natural and synthetic systems, and our understanding of them is still very rudimentary.*

ENERGY FRONTIER RESEARCH CENTERS

## Energy Frontier Research Centers

To implement the collective recommendations of these twelve workshops, the Office of Basic Energy Sciences announces a new initiative: the Energy Frontier Research Centers (EFRCs). The EFRC awards are expected to be in the $2–5 million range annually for an initial five-year period. A Funding Opportunity Announcement (FOA) in 2008 requests applications from the scientific community for the establishment of the initial suite of EFRCs. It is anticipated that approximately $100 million will be available for multiple EFRC awards starting in FY 2009.

### *Distinguishing Attributes*

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. As such, the EFRCs will strengthen and complement the existing portfolio of single-principal investigator and small group research projects currently supported within BES core research areas. An EFRC will have the following characteristics:

- The research program is at the forefront of 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 ).

- The research program addresses one or more of the energy challenges described in the ten BES workshop reports in the *Basic Research Needs* series (http://www.sc.doe.gov/bes/reports/list.html).

- The program is balanced and comprehensive and, as needed, supports experimental, theoretical, and computational efforts and develops new approaches in these areas.

- The program provides opportunities to inspire, train, and support leading scientists of the future who have an appreciation for the global energy challenges of the 21st century.

- The center leadership communicates effectively with scientists of all disciplines and promotes awareness of the importance of energy science and technology.

- There is a comprehensive management plan for a world-leading program that encourages high-risk, high-reward research. The Center's management plan demonstrates that the whole is substantially greater than the sum of the individual parts.

## *EFRC's Awards Process*

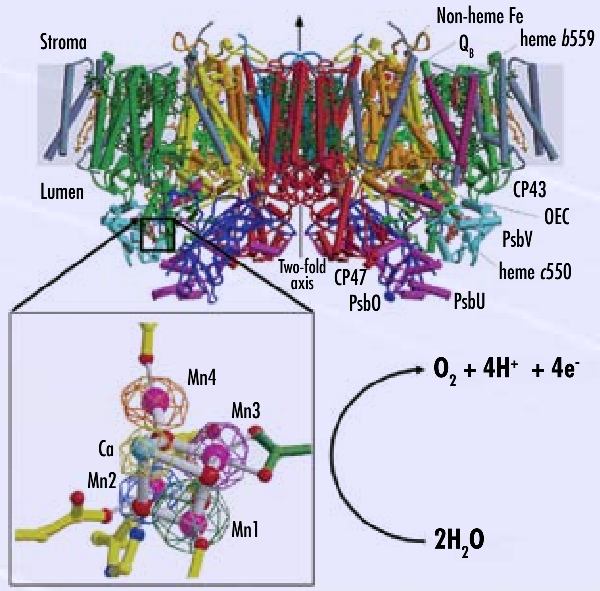
A number of EFRC awards will be initiated in FY 2009 based on an open competition among academic institutions, DOE laboratories, and other institutions. Research activities may be sited at universities, at DOE laboratories, or in joint university-laboratory collaborations. The EFRC awards are expected to be in the $2–5 million range annually for an initial five-year period. A Funding Opportunity Announcement (FOA) in 2008 requests applications from the scientific community for the establishment of the initial suite of EFRCs. It is anticipated that approximately $100 million will be available for multiple EFRC awards. As the EFRC program matures, it is anticipated that EFRC competitions will be held every two or three years and that renewal submissions will be openly competed for by new submissions. Out-year funding is subject to satisfactory progress in the research and the availability of funding appropriations. While capital investment in instrumentation and infrastructure are expected as part of the EFRC awards, usage and leverage of existing facilities, including the BES user facilities, is encouraged. This announcement, updates, and further information on the FOA will be available through a link on the BES home page (http://www.sc.doe.gov/bes/).

## *Example EFRC Research Focus Areas*

A few examples of science areas that would respond to the EFRC solicitation are given below. These are intended to be examples only. The intent of the program is to allow for maximum flexibility within the broad guidelines given above. We are particularly interested in tapping the imagination and creativity of the scientific community to address the fundamental questions of how nature works and to harness this new knowledge for some of our most critical 21st century energy challenges.

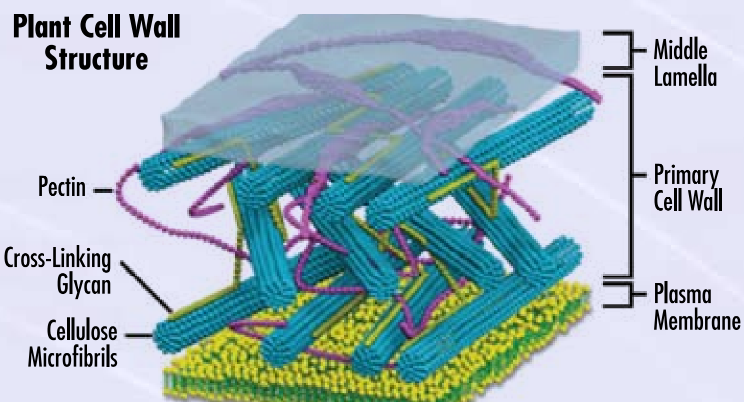
## Direct conversion of solar energy to electricity and chemical fuels

Learning to direct and control materials and chemical processes at the level of electrons, where the laws of quantum mechanics rule, would pave the way for essentially new quantum control impacting catalysis, photochemistry, molecular biology, and device physics that are the foundational pieces in solar energy conversion. Powerful new methods of nanoscale fabrication, characterization, and simulation—using physical, chemical and biological tools that were not available as few as five years ago—create new opportunities for understanding and manipulating the molecular and electronic pathways of solar energy conversion. Specific areas include coaxing cheap materials for superior performance; new paradigms for solar cell design; photocatalytic processes for inexpensive, efficient conversion; and bio-inspired methods for self-assembly of molecular components into functional self-regulating and self-repairing systems for solar fuel production.




*The natural photosynthetic system of a green leaf (top) provides the biological inspiration for artificial systems designed to do what a plant does: split water into molecular oxygen and hydrogen fuel. By mimicking the light-active reaction center (detail at bottom), scientists hope to duplicate nature's miracle of a self-regulating and self-repairing solar fuel generator. (Derived from Figures 1 and 5 of K.N. Ferreira, T.M. Iverson, K. Maghlaoui, J. Barber, and S. Iwata, "Architecture of the photosynthetic oxygen-evolving center,"* Science ***303****, 1831-1838 [2004].)*

## Understanding of how biological feedstocks are converted into portable fuels[1]




*A plant cell wall, which is the raw material for cellulosic biofuels, is a complex nanostructure of polymers that is not completely understood at the molecular level. Sophisticated physical and chemical characterization of the plant cell wall may enable vastly improved methods for production of cellulosic biofuels. (From* Basic Research Needs: Catalysis for Energy*, Figure 36, prepared by Michael W. Davidson, Florida State University [http://micro.magnet.fsu.edu/cells/plants/cellwall.html])*

Biological systems are the proof-of-concept for what can be physically achieved by nanotechnology. Consider the ease with which biological systems transform and store energy or their ability to self-repair and to adapt to changing external conditions. The way in which energy, entropy, and information are manipulated within the nanosystems of life provide lessons on how to develop similarly sophisticated energy technologies. This entails research in light harvesting, exciton transfer, charge separation, transfer of reductant to carbon dioxide as well as carbon fixation, storage and conversion. Specific areas might include molecular-scale characterization of the physical structure and chemical properties of plant cell wall materials with the aim of circumventing the need

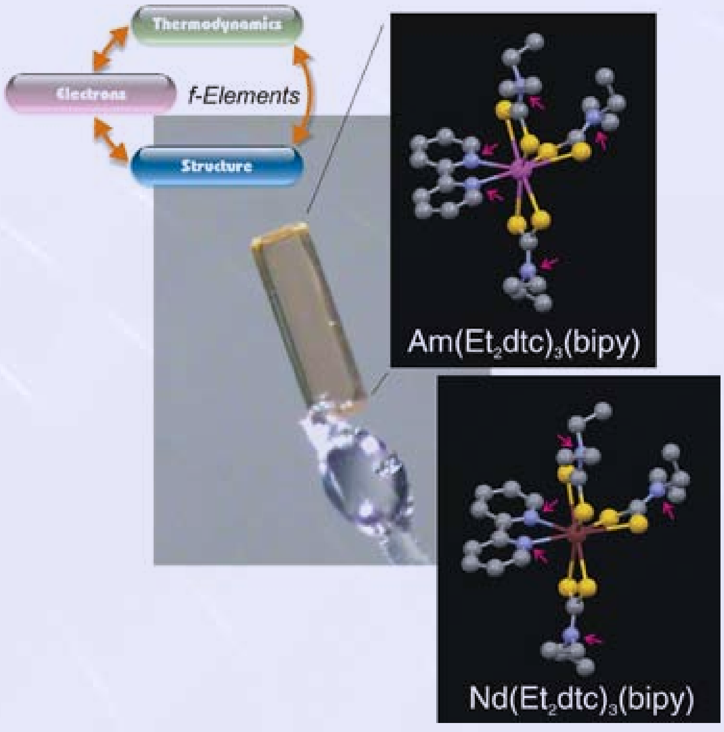
*[1] Within the Office of Science, both the BES and the Biological and Environmental Research (BER) programs' biofuels research involve the direct biological conversion of solar energy into chemically stored fuels. However, there are distinct differences. BES focuses on the conversion mechanisms, emphasizing the associated physical and chemical processes, and their coupling with bio- and biomimetic approaches. In contrast, BER focuses on the biological processes, with an emphasis on genomics, metabolic engineering, systems biology, and biotechnological tools for scalable biofuels production.*

for extensive pre-treatment and biological hydrolysis to sugars (saccharification), which are current bottlenecks in cellulosic biofuel production. Other areas include development of new and improved catalytic conversion processes that are far more robust than enzymatic systems for the conversion of plant polymers to fuels. A fundamental understanding of biomass deconstruction, either through high-temperature pyrolysis or low-temperature catalytic conversion, is sought along with the development of new catalysts for targeted transformations of biomass-derived molecules into fuels. The accompanying image illustrates the complex plant cell structure that needs to be characterized and controlled at the molecular level. Developing a molecular-scale understanding of deconstruction and conversion of biomass products to fuels would contribute to the development of optimal processes for particular biomass sources. Knowledge of how catalyst structure and composition affect the kinetics of elementary processes could lead to new catalysts with properties adjusted for maximum activity and selectivity for high- and low-temperature processing of biomass.

## A new generation of radiation-tolerant materials and chemical separation processes for fission applications

By designing and perfecting atom- and energy-efficient synthesis, one can create a paradigm shift in the discovery and design of new chemical assemblies and materials that are mechanical strong; light weight; and resistant to corrosion, decay, or failure in extreme conditions of temperature, pressure, radiation, or chemical exposures encountered in fission applications.

Key research includes: foundational research in chemistry and physics of actinides and their fission products; a new generation of actinide separations processes with improved efficiency, selectivity, cost-effectiveness, and waste minimization; first-principles design and understanding of materials with improved radiation and corrosion resistance at elevated temperatures; microstructural design and predictive models to mitigate long-time degradation behavior in these materials; characterization, theory, and computer models for decades-to-centuries performance for fission waste hosts; and solution and interfacial behavior of chemical separations systems under extreme radiation flux and elevated temperatures.

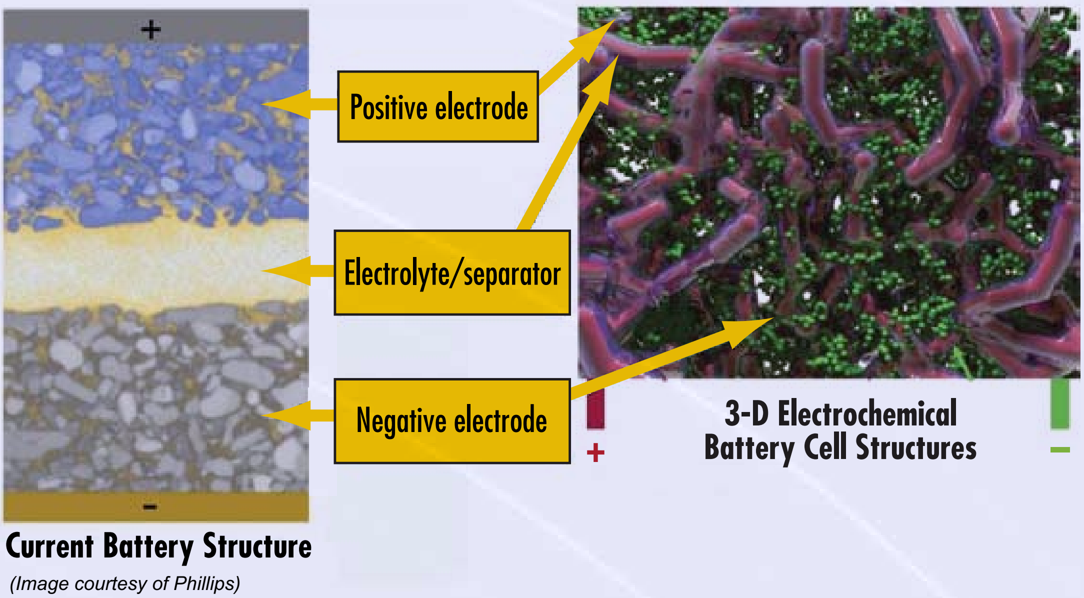



*Understanding the chemistry of the actinides is an essential foundation to the design and implementation of a broad range of advanced fission technologies. Actinide chemistry is often dominated by the unusual chemical bonding properties of f electrons. The photograph shows a single crystal of an americium-nitrogen complex with a molecular structure (top right) that appears similar to the neodymium complex (bottom right). However, the americium ion (magenta) has "delocalized" 5f electrons that bond strongly with nitrogen atoms (lavender with arrows), whereas the neodymium ion (brown) has the same radius but more "localized" 4f electrons that are much less effective at bonding with nitrogen atoms. (Prepared by Mark Jensen, Argonne National Laboratory)*

## Addressing fundamental knowledge gaps in energy storage

Without effective electrical energy storage, renewable—yet intermittent—sources of energy such as wind and solar will not be able to significantly displace fossil, nuclear, and other conventional energy sources used for generating electricity for the power grid. Similarly, current battery technologies are limited, making plug-in hybrid or all-electric cars prohibitively costly and insufficient to meet consumer demands. Long-term, fundamental research in electrical energy storage will be needed to accelerate the pace of scientific discoveries and to see transformational advances that bridge the gaps in cost and performance, separating current technologies and those required for future utility and transportation needs.

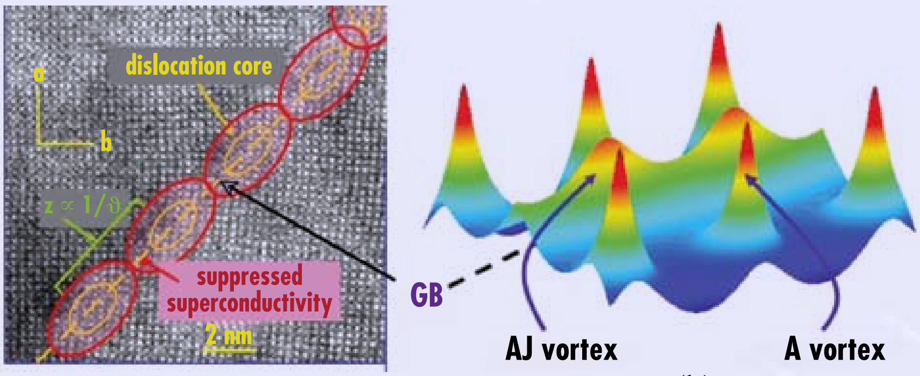
For example, by mastering energy balance on the nanoscale through harvesting the large number of forces that are often operating simultaneously, such as electrostatic attraction and repulsion, chemical bonding, surface tension, and random forces from environmental fluctuations, a wide variety of structures can be assembled for 3-D architectures, as illustrated in the image below, with multi-functionalities in energy storage unsurpassed by any given existing technologies. Other research areas include new capabilities to "observe" dynamic composition and structure; novel electrolytes with high conductivity over a broad temperature range and long-term stability; and theory, modeling, and simulation that integrate methods at different time and length scales.




*Battery structures: conventional, requiring discrete segregated elements (left) and an integrated cell enabled by nanoscale materials (right).* (From Basic Research Needs: Electrical Energy Storage*, Figure 5, prepared by J.W. Long, B. Dunn, D.R. Rolison, and H.S. White, published in "Three-dimensional battery architectures,"* Chem. Rev. ***104****, 4463–4492 [2004].)*

## Transforming energy utilization and transmission

At the heart of nanoscale behavior, one often finds emergent phenomena, in which a complex outcome emerges from the correlated interactions of many simple constituents. By understanding the fundamental rules of correlations and emergence and then by learning how to control them, we could produce, for example, an entirely new generation of energy utilization and transmission processes, such as in phase change materials for thermal energy conversion, strong light-matter interaction and collective charge behavior for light emission nearing theoretical efficiency, and radically different combustion chemistry of alternative fuels. Understanding the emergent behavior of materials and chemical reactivity at the nanoscale offers remarkable opportunities in a broad arena of applications including solid-state lighting, electrical generators, clean and efficient combustion of 21st century transportation fuels, catalytic processes for efficient production and utilization of chemical fuels, and superconductivity for resistance-less electricity transmission.



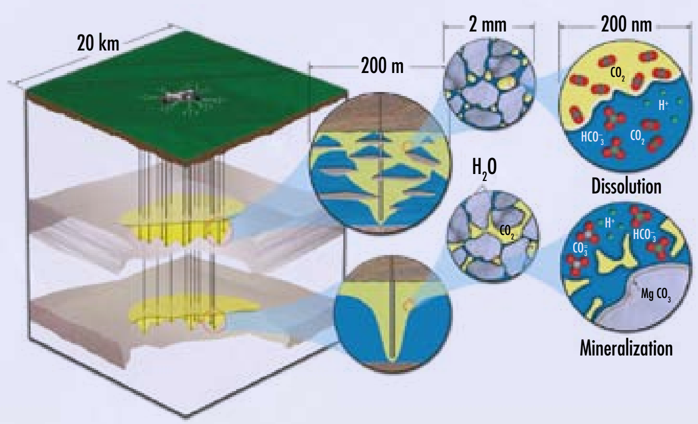

(a) (b)

*One of superconductivity's two composite phenomenon building blocks, so-called Abrikosov vortices, depends upon the crystal structure's nanoscale details. A chain of crystal dislocations can suppress a superconductor's current-carrying ability (a), which is understood on the basis of a theoretical calculation showing the associated complex emergent behavior (b). (From* Basic Research Needs for Superconductivity, *Figure 8.)*

## Science-based geological carbon sequestration

All naturally and most human-induced phenomena occur in systems that are away from the equilibrium in which the system would not change with time. If we can understand system effects that take place away—especially very far away—from equilibrium and learn to control them, it could yield dramatic new carbon capture technologies and enable new strategies for sequestering carbon to mitigate environmental damage.

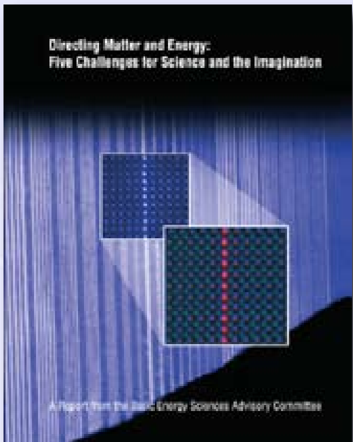
Key research areas involve new membranes and separations of carbon dioxide from process streams at high temperature and pressure; understanding geochemical processes relevant to the dimensions of subsurface sequestration sites with realistic geological formations chemistry; developing critical geophysical measurement techniques for remote probing and tracking; developing fluid-flow measurement approaches and simulation tools that can link chemical and physical processes at multiple scales; and advanced measurement and modeling verification at field sites.




*Storage of $CO_2$ in an underground formation (left) represents a complex, highly nonequilbrium system with important features at a multitude of spatial scales. The central insets show $CO_2$ as a mobile phase (lower) and as a trapped residual phase (upper) at a scale of 200 meters. The insets on the right show the nanometer scale mechanisms of $CO_2$ trapping — dissolution (upper) and mineralization (lower). (From* The Future of Coal: Options for a Carbon-Constrained World, *Massachusetts Institute of Technology, p. 175 [2007].)*

# Appendix: Scientific Workshop Reports

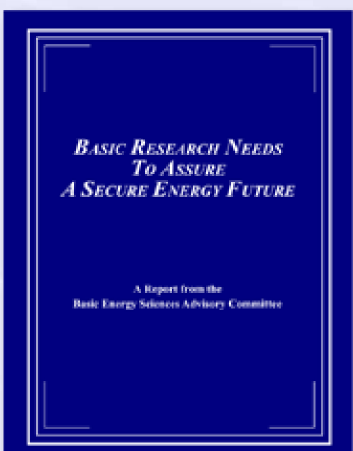
Energy Frontier Research Centers are based on a scientific knowledge base of energy-relevant research that has been articulated through the recent development of a series of twelve workshop reports (http://www.sc.doe.gov/bes/reports/list.html).




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

This Basic Energy Sciences Advisory Committee (BESAC) Grand Challenges report identifies the most important scientific questions and science-driven technical challenges facing BES and describes the importance of these challenges to advances in disciplinary science, to technology development, and to energy and other societal needs. Acquiring the ability to direct and control matter all the way down to molecular, atomic, and electronic levels will require fundamental new knowledge in several critical areas. This report was commissioned to define those knowledge areas and the opportunities that lie beyond. Five interconnected Grand Challenges were identified with recommendations for what must be done to meet them.

Modern science stands at the beginning of what might seem by today's standards to be an almost magical leap forward in our understanding and control of matter, energy, and information at the molecular and atomic levels. Atoms, and the molecules they form through the sharing or exchanging of electrons, are the building blocks of the biological and non-biological materials that make up the world around us. In the 20th century, scientists continually improved their ability to observe and understand the interactions between atoms and molecules that determine material properties and processes. Now, scientists are positioned to begin directing those interactions and controlling the outcomes on a molecule-by-molecule and atom-by-atom basis, or even at the level of electrons. This ability will help us meet some of humanity's greatest needs, including the need for abundant, clean, and cheap energy.




## Basic Research Needs to Assure a Secure Energy Future

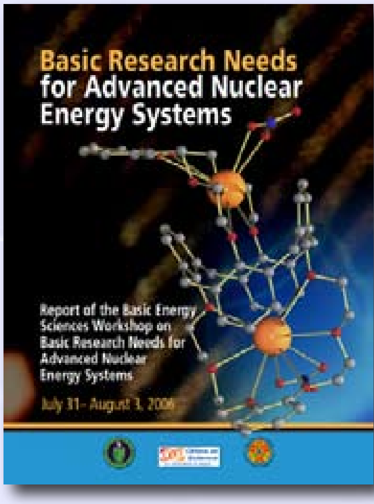
Current projections estimate that the energy needs of the world will more than double by the year 2050. This is coupled with increasing demands for "clean" energy—sources of energy that do not add to the already high levels of carbon dioxide and other pollutants in the environment. These enormous challenges cannot be fully met by existing technologies, and scientific breakthroughs will be required to provide reliable, economic solutions for our future energy security.

This seminal workshop report identified the broad basic research directions that will help provide the major scientific discoveries necessary for major technological changes in the largest industries in the world—those responsible for energy production and use.

The findings of this 2003 report gave birth to a series of ten follow-up Basic Research Needs workshops over the next five years, which together attracted more than 1,500 participants from universities, industry, and Department of Energy laboratories.  These reports provide in-depth analyses on how the work of the scientific community can further our nation's most challenging energy missions.

Together, these workshop reports highlighted the remarkable scientific journey that took place during the past few decades. The resulting scientific challenges, which no longer were discussed in terms of traditional scientific disciplines, described a new era of science — an era in which materials functionalities would be designed to specifications and chemical transformations would be manipulated at will.

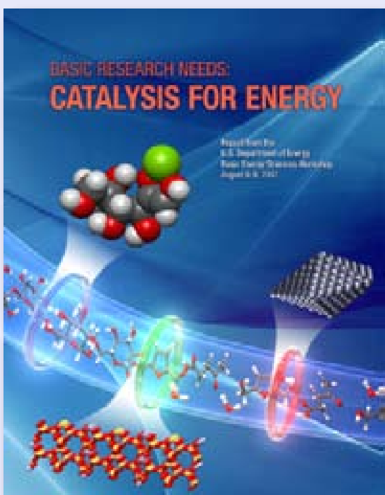
Over and over, the recommendations from the workshops described similar themes — that in this new era of science, we would design, discover, and synthesize new materials and molecular assemblies through atomic scale control; probe and control photon, phonon, electron, and ion interactions with matter; 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, and those skilled in applied mathematics and computer science.




## Advanced Nuclear Energy Systems

Many studies project significant growth in the utilization of nuclear power as a source of carbon dioxide-free energy over the next decades. Projected growth in nuclear power has focused increasing attention on the replacement of the once-through nuclear fuel cycle with closed nuclear fuel cycles and the permanent disposal of a much smaller amount of nuclear waste.

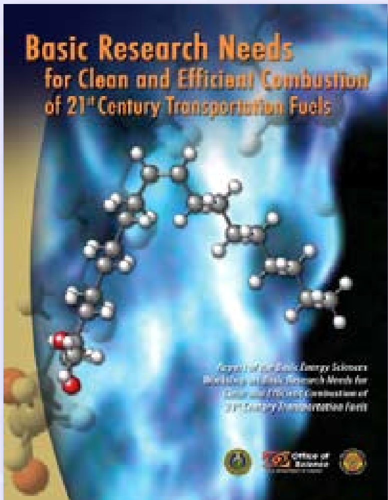
The workshop identified new, emerging, and scientifically challenging areas in materials and chemical sciences that have the potential for significant impact on advanced nuclear energy systems. The performance of materials and chemical processes under extreme conditions of radiation fields and temperature present a fundamental challenge to understanding and controlling chemical and physical phenomena in multi-component systems from femtoseconds to millennia, at temperatures to 1000 ºC, and under high radiation doses. Nanoscale characterization methods are needed to design materials with radiation, temperature, and corrosion resistance. First-principles approaches are needed to describe 5f-electron (actinide) systems, to design molecules for separations, and to explain failure mechanisms of materials. Dynamic measurements are required to understand fundamental physical and chemical phenomena, especially at interfaces, in multi-component systems, and at the nanoscale and mesoscale in solution. New multiscale approaches are needed to integrate this knowledge into accurate models of relevant phenomena and complex systems across multiple length and time scales. These themes define a science-based approach to the development of materials and chemical processes for advanced nuclear energy systems.




## Catalysis for Energy

As the domestic reserves of petroleum and natural gas decline, the volumes of imported fuels grow, and the environmental impacts resulting from fossil fuel combustion become severe, our nation must earnestly reassess our future chemical energy sources. Catalysis—the essential technology for accelerating and directing chemical transformation—is key to realizing environmentally friendly, efficient and economical processes for the conversion of fossil and renewable or alternative energy feedstocks.

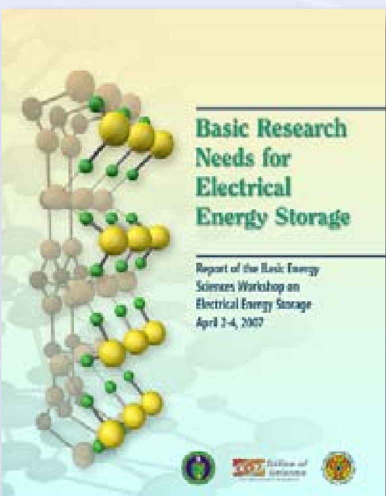
The workshop examined basic research needs to maximize the potential for new catalytic discoveries in three specific areas according to source: bio-derived chemicals, heavy fossil-derived chemicals, and end-product (such as carbon dioxide and water) reconversion. The grand challenge identified at the core of all of these areas was to achieve detailed mechanistic understanding of catalytic dynamics for complex heavy molecular mixtures, bio-derived species, and solid nanostructures and interfaces. Such understanding would allow scientists to build effective catalysts with atom-by-atom precision and convert complex reactants to energy-storing products with molecular precision. The means to resolve this challenge is several-fold: creating new and expanding existing fundamental theories of chemical kinetics that effectively take into account the dynamics and statistical fluctuations of structurally complex and diverse feedstocks; creating and advancing instrumentation that permits real-time high-resolution chemical imaging of reacting species and catalysts; and synthesizing new and more complex catalyst structures that exploit multifunctionality and versatility in order to guide reactions through highly selective pathways.




## Clean and Efficient Combustion of 21st Century Transportation Fuels

Our nation's nearly total dependence on light, sweet crude oil for our transportation fuels will draw to a close over the coming decades as finite resources are exhausted. New fuel sources from renewable biomass or non-traditional fossil reserves (oil shale, tar sands, and coal), with differing and variable chemical characteristics, are emerging to replace crude oil. As these new fuel streams enter the market, a series of new engine technologies are also under development, promising improved efficiency and cleaner combustion. To date, however, a coordinated strategic effort to match future fuels with evolving engines is lacking.

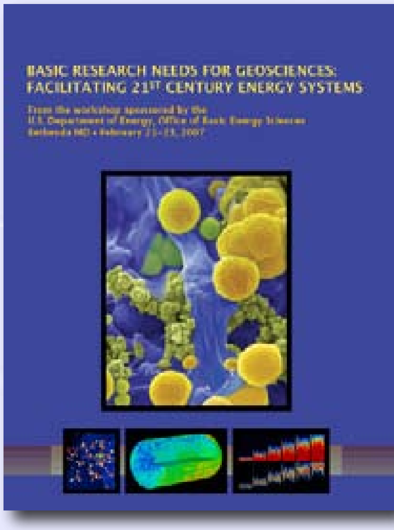
This workshop was charged with exploring basic research needs in the areas of gas-phase chemistry, combustion diagnostics, and combustion simulation that will enable the use of transportation fuels derived from non-traditional sources (oil shale, tar sands, coal, biomass) in a manner that optimizes engine efficiency and minimizes pollutant formation. Eight priority research directions were identified, two of which were devoted to a focus on engines or fuels and were similar in their strategy of working backward from technology drivers to scientific research needs. A third panel explored crosscutting science themes and identified critical gaps in our scientific understanding of 21st century fuel combustion. The workshop identified a single, overarching grand challenge: the development of a validated, predictive, multi-scale, combustion modeling capability to optimize the design and operation of evolving fuels in advanced engines for transportation applications. The workshop produced a keen sense of urgency and opportunity for the development of revolutionary combustion technology for transportation based upon fundamental combustion science.




## Electrical Energy Storage

The projected doubling of world energy consumption within the next 50 years, coupled with the growing demand for low- or even zero-emission sources of energy, has brought increasing awareness of the need for efficient, clean, and renewable energy sources. Energy based on electricity generated from renewable sources, such as solar or wind, offers enormous potential for meeting future energy demands. However, practical use of large scale solar- or wind-based electrical generation requires electrical energy storage (EES) systems to level their cyclic nature. In addition, greatly improved EES systems are needed to replace today's hybrid electric vehicles with plug-in hybrids or all-electric vehicles.

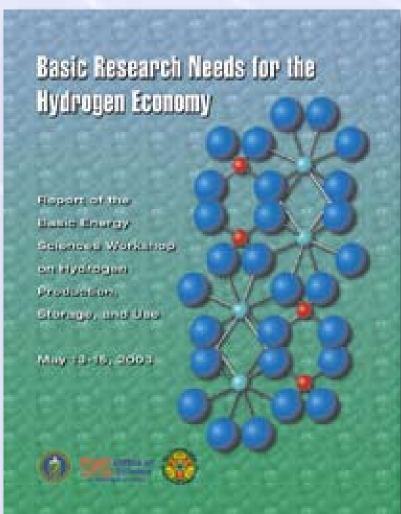
Fundamental performance limitations of energy storage systems are rooted in the constituent materials making up an EES device, and novel approaches are needed to develop multifunctional EES materials that offer new self-healing, self-regulating, failure-tolerant, impurity-sequestering, and sustainable characteristics. The discovery of novel nanoscale materials with architectures tailored for specific performance offer particularly exciting possibilities for the development of revolutionary three-dimensional architectures that simultaneously optimize ion and electron transport and capacity. New capabilities are also needed to "observe" the dynamic composition and structure at an electrode surface, in real time, during charge transport and transfer processes. New *in situ* photon- and particle-based microscopic, spectroscopic and scattering techniques with time resolution down to the femtosecond range and spatial resolution spanning the atomic and mesoscopic scales are needed to meet this challenge. Research to formulate a predictive knowledge of structural and functional relationships based upon multiscale integrating theory-based methods at different time and length scales can effectively complement experimental efforts to provide insight into mechanisms, predict trends and identify new materials. With such underpinning knowledge, wholly new concepts in rational materials design can result in EES systems capable of storing higher energy densities with long cycle lifetimes.




## Geosciences: Facilitating 21st Century Energy Systems

The fundamental geosciences challenge is to understand the subsurface well enough to be able to predict its response to anthropogenic perturbations over societally relevant time periods. Continued use of fossil energy in a greenhouse-gas-constrained world will require the capture and sequestration of a substantial fraction of the produced carbon dioxide in deep subsurface storage sites. Nuclear energy usage could reduce $CO_2$ generation, but nuclear power results in spent nuclear fuel and other radioactive materials that also must be stored underground. This report describes the scientific challenges associated with these technology options. New information is needed on the properties and processes associated with complex and heterogeneous subsurface mineral assemblages comprising porous rock formations, and the equally complex fluids that may reside within and flow through those formations.

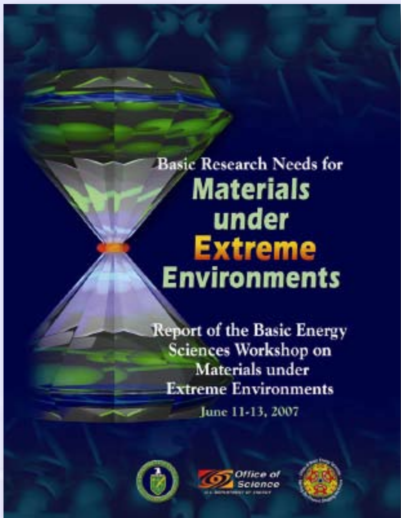
This report describes the scientific challenges associated with underground storage options for carbon dioxide and radioactive waste. New information is needed on the properties and processes associated with complex and heterogeneous subsurface mineral assemblages comprising porous rock formations, and the equally complex fluids that may reside within and flow through those formations. The relevant physical and chemical interactions occur on spatial scales that range from those of atoms, molecules, and mineral surfaces, up to tens of kilometers, and time scales that range from picoseconds to millennia. To predict with confidence the transport and fate of either $CO_2$ or the various components of stored nuclear materials, we need to learn to better describe fundamental atomic, molecular, and biological processes, and to translate those microscale descriptions into macroscopic properties of materials and fluids. We also need fundamental advances in the ability to simulate multi-scale systems as they are perturbed during sequestration activities and for very long times afterward, and to monitor those systems in real time with increasing spatial and temporal resolution. The ultimate objective is to predict accurately the performance of the subsurface fluid-rock storage systems, and to verify enough of the predicted performance with direct observations to build confidence that the systems will meet their design targets as well as environmental protection goals.




## Hydrogen Economy

The coupled challenges of the increasing world's energy needs and demands for "clean" energy sources that do not add more carbon dioxide and other pollutants to the environment have resulted in increased attention worldwide to the possibilities of a "hydrogen economy" as a long-term solution for a secure energy future. The hydrogen economy offers a grand vision for energy management in the future. Its benefits are legion, including an ample and sustainable supply, flexible interchange with existing energy media, a diversity of end uses to produce electricity through fuel cells or to produce heat through controlled combustion, convenient storage for load leveling, and a potentially large reduction in harmful environmental pollutants.

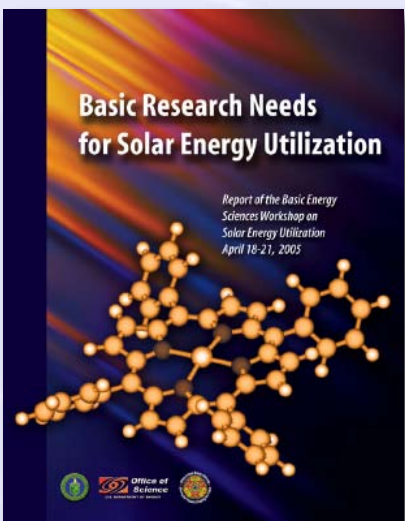
The essence of this report is captured in six cross-cutting research directions that were identified as being vital for enabling the dramatic breakthroughs to achieve lower costs, higher performance, and greater reliability that are needed for a competitive hydrogen economy: catalysis; nanostructured materials; membranes and separations; characterization and measurement techniques; theory, modeling, and simulation; and safety and environmental issues.




## Materials under Extreme Environments

Materials are recognized as being central to every energy technology, and future energy technologies will place increasing demands on materials performance with respect to extremes in stress, strain, temperature, pressure, chemical reactivity, photon or radiation flux, and electric or magnetic fields. Hence, it is not surprising that the failure of materials is a principal bottleneck for developing future energy technologies. New fundamental research of materials under extreme conditions will have a major impact on the development of numerous integrated technologies that can meet future requirements for abundant, affordable, and clean energy.

Reaching the intrinsic limit of materials performance is a key challenge, and solutions to this challenge require new understanding regarding the most fundamental atomic and molecular origins of material failure. In particular, ultra-high spatial and ultrafast temporal resolution characterization tools are needed to observe and follow the initiation and evolution of atomic-scale to cascading macroscale damage events. Complementary advanced computational capabilities to simulate and predict multiscale damage from atomic to macroscopic dimensions are also needed. Such new understanding of damage and failure will underpin research to discover how atomic and molecular structures could be manipulated in a predicable manner to enable development of new materials having an extraordinary tolerance to function within an extreme environment without property degradation, or even with the ability for self-repair.

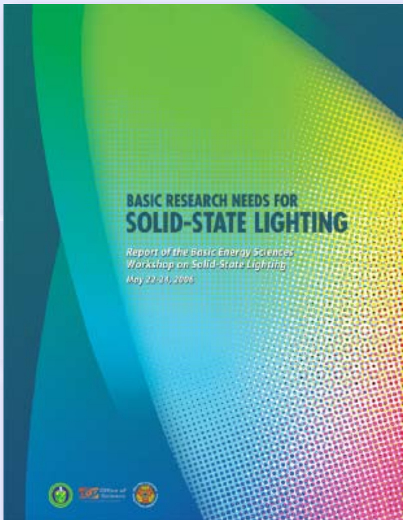



## Solar Energy Utilization

More energy from sunlight strikes the Earth in one hour than all the energy consumed on the planet in one year. Yet, we currently exploit this solar resource through solar electricity at less than one percent of the world's electricity needs, and through solar-derived fuel from biomass at less than two percent of the world's energy. Finding a sufficient supply of clean energy for the future is one of society's most daunting challenges and incremental improvements in existing energy networks will not be adequate to meet this demand in a sustainable way. Solar energy and its enormous undeveloped potential define a grand challenge in energy research. In response to that challenge, this workshop identified the key scientific problems and research directions that will enable efficient and economic use of the solar resource to provide a significant fraction of global primary energy by the mid-21st century.

Solar energy conversion systems fall into three categories according to their primary energy product: solar electricity, solar fuels, and solar thermal systems. Although large technological barriers lay between the present and this mid-21st century primary energy goal, the workshop identified thirteen priority research directions with high potential for producing scientific breakthroughs, ones that could dramatically advance solar energy conversion to electricity, fuels, and thermal power.

## Solid-State Lighting




In 2001, twenty-two percent of the nation's electricity, equivalent to eight percent of the nation's total energy, was used for artificial light. The cost of this energy to the consumer was roughly $50 billion per year or approximately $200 for every person living in the U.S. The cost of this energy to the environment was approximately 130 million tons of carbon emitted into our atmosphere, or about seven percent of all the carbon emitted by the U.S. Our increasingly precious energy resources and the growing threat of climate change demand that we reduce the energy and environmental cost of artificial lighting, an essential and pervasive staple of modern life. If a fifty percent-efficient technology were to exist and be extensively adopted, it would reduce energy consumption in the U.S. by about 620 billion kilowatt-hours per year by the year 2025 and eliminate the need for about seventy nuclear plants, each generating a billion watts of power. Solid state lighting (SSL) modalities present an opportunity to achieve tremendous advances in energy efficiency.

Broad areas of discovery research and scientific inquiry were identified as required SSL groundwork, condensed in the following two primary challenges. One broad research challenge aims to change the very paradigm by which SSL structures are designed, moving from serendipitous discovery towards rational design. The other challenge aims to understand and control the microscopic pathways through which losses occur as electrons produce light, which is identified as a primary roadblock to SSL. By discovering and controlling the materials and nanostructure properties that mediate the competing conversion of electrons to light and heat, the challenge of converting every injected electron into useful photons will be addressed. The anticipated results are ultra-high-efficiency light-emitting materials and nanostructures, and a deep scientific understanding of how light interacts with matter, with broad impact on science and technology areas beyond SSL.

## Superconductivity


As an energy carrier, electricity has no rival with regard to its environmental cleanliness, flexibility in interfacing with multiple production sources and end uses, and efficiency of delivery. However, the challenge facing the electricity grid to provide abundant, reliable power will soon grow to crisis proportions. Incremental advances in existing grid technology are not capable of solving the bottlenecks to power transmission. Revolutionary new power transmission and control solutions based on superconductors can solve this crisis by increasing the grid's capacity, efficiency, stability and reliability as they are uniquely capable of carrying current without loss, mediating overcurrents intrinsically while providing instantaneous power regulation.

Advancing the state-of-the-art in superconductivity presents a formidable research challenge, as its nature is one of fundamental science puzzles in a profusion of intriguing effects. A central challenge with the biggest impact is the need to understand the fundamental mechanisms of high-temperature superconductivity. This is difficult precisely because the mechanisms are entangled with many anomalous normal state effects. Another primary scientific opportunity is rooted in nanoscale phenomenon as superconductivity's two composite building blocks have dimensions ranging from a tenth of a nanometer to a hundred nanometers. Unraveling superconductivity's mechanism with the promise of nanoscale fabrication, characterization, and simulation will provide a pathway for the rational design of and production of functional superconducting materials required for next-generation grid technology.


Basic Research Needs for Advanced Nuclear Systems
BASIC RESEARCH NEEDS CATALYSIS FOR ENERGY
Basic Research Needs for Clean and Efficient Combustion of 21st Century Transportation Fuels
Basic Research Needs for Electrical Energy Storage
BASIC RESEARCH NEEDS FOR GEOSCIENCES: FACILITATING 21st CENTURY ENERGY SYSTEMS
Basic Research Needs for Materials under Extreme Environments
Basic Research Needs for Solar Energy Utilization
BASIC RESEARCH NEEDS FOR SOLID-STATE LIGHTING
BASIC RESEARCH NEEDS FOR SUPERCONDUCTIVITY

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