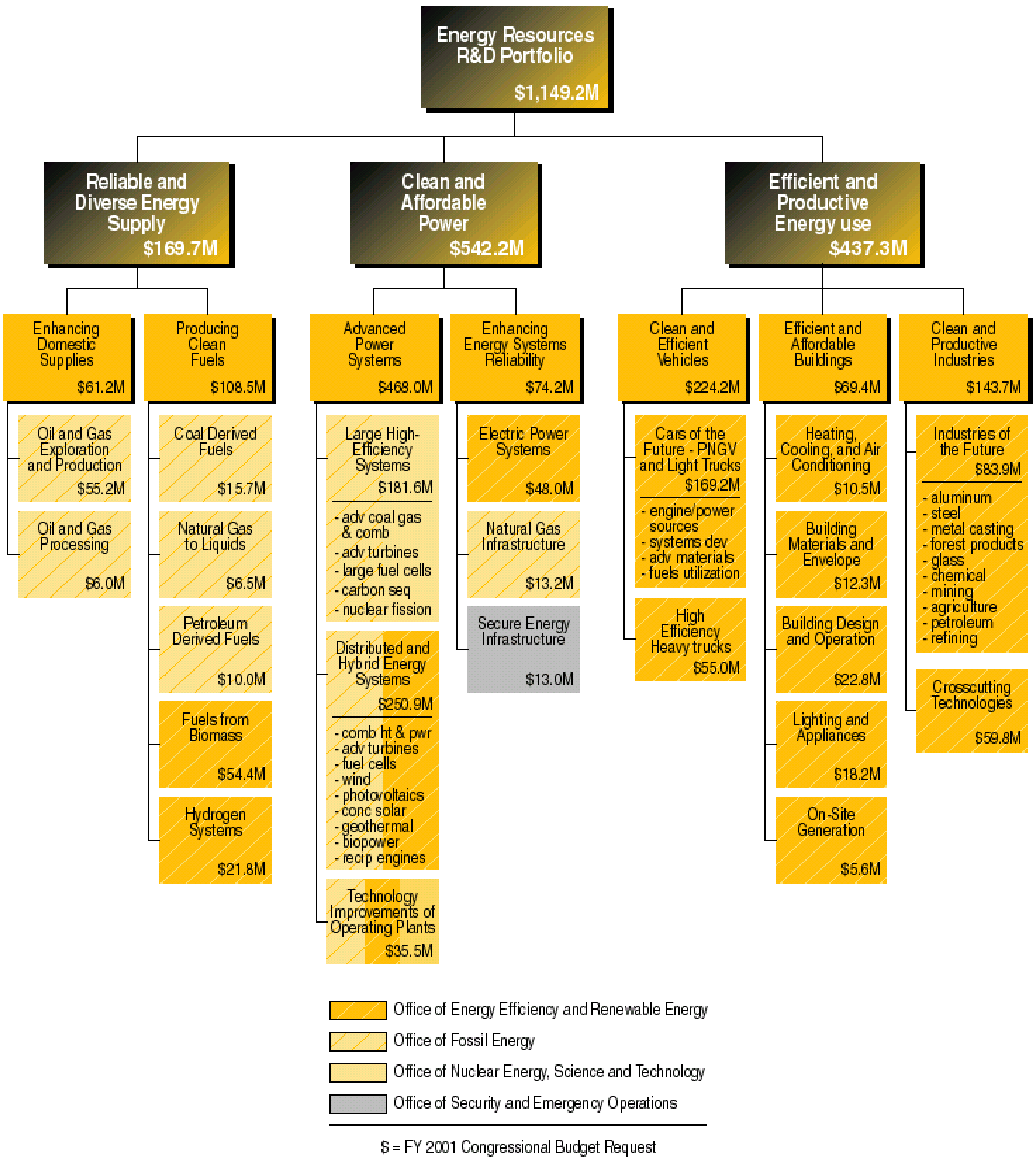
Chapter 10
Basic Science



Chapter 10
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Overview

The Department of Energy maintains a sizeable portfolio of basic research that underpins DOE's applied R&D missions and explores broad frontiers in fundamental science, leading the Nation in the basic energy and physical sciences. Overall, this chapter addresses the contribution of basic science to the energy R&D mission, that is to say, the contributions of the DOE's Office of Science (SC) to applied energy R&D programs. A companion document to the overall Energy R&D Portfolio addresses the issues and implications of the Department's broader Science Portfolio.

In support of its basic science mission, DOE manages the most extensive and advanced complex of scientific facilities in the world. Such facilities, managed by SC, include powerful accelerators for high energy and nuclear physics, light and neutron beam facilities for the natural and life sciences, electron beam microcharacterization centers, multidisciplinary mission centers, and single purpose research facilities. Beyond DOE-sponsored research, the Department provides access to these facilities for the Nation's professors, students, and public and private-sector researchers.

Within the Department, the basic science programs are funded within SC at a total of $2.7 billion in FY 1999. This budget supports basic science, research facilities, and related infrastructure.

In pursuit of energy goals, research supports, as well as draws from, a broad spectrum of science disciplines. Most of these disciplines contribute directly to the applied energy R&D mission of the Department. These include:

- materials science
- environmental sciences
- fusion/plasma sciences
- energy technology research
- chemical sciences
- high energy and nuclear physics
- biological and biomedical sciences
- computational and math sciences
- engineering sciences
- geosciences
- energy biosciences

The National Laboratories, universities/colleges, and the private sector perform the research.

A distinguishing, general feature of basic science is that it is primarily knowledge rather than application driven. That is to say, one of its main purposes is to explore the complex phenomenon and processes that define our physical world, to determine what factors influence them, and to understand how we may ultimately control them. At this basic level, discoveries and insights usually have broad-reaching, diverse implications for many applied R&D and technology development programs, not just one.

Support for Energy R&D

Although most of the Department's basic science research has broad-based, generic implications for technology programs, some of this research aligns more strongly with particular energy technology applications, depending on the questions and phenomenon that the science addresses and the challenges inherent to the applied R&D area. For example, discoveries in the science of lightweight, high-strength materials, as well as advanced material joining techniques and properties align strongly with applications for next generation, efficient vehicles. To add perspective on how basic science supports applied energy R&D applications, additional examples are provided below in each of the seven other energy R&D areas:

- Enhancing Domestic Supplies.
- Producing Clean Fuels.
- Advanced Power Systems.
- Enhancing Utility Infrastructure.
- Clean and Efficient Vehicles.
- Efficient and Affordable Buildings.
- Clean and Productive Industries

Note that these examples are just that, examples. They are intended to illustrate the strong link that exists between the Department's basic science programs and innovation in DOE's applied energy R&D programs.

Enhancing Domestic Supplies

Examples of basic science that support Enhancing Domestic Supplies are provided below. Most of this research is carried out by the Office of Basic Energy Sciences, the Office of Biological and Environmental Research, and the Office of Computational and Technology Research.

- *Geosciences:* Basic research in Geosciences focuses on improving the level of understanding necessary for advances in, and choices among, current and emerging energy and environmental technologies. Primary research focus areas are geochemistry, geophysics, geomechanics, and hydrology. Additionally, research in chemistry focuses on fundamental molecular-level understanding of chemical interactions and chemical reactions, the development of new analytical tools and methods, and the physical and chemical interactions forming the bases for new membranes for separation processes. These programs also provide the fundamental thermal and physical properties that are the bases of all engineering applications. Research in materials sciences provides the knowledge for new materials impacting domestic supplies in every area from advanced materials for drill bits to new-concept storage methods. More directly, the basic research within geosciences efforts focuses on:

  – Improved fundamental research on mineral-fluid interactions will provide a better understanding of the origin, migration and localization of oil and gas resources, the location and management of geothermal resources, and the control of energy-related wastes in the vadose and saturated groundwater zones.

– New fundamental thermodynamic and physical property information on rocks, minerals, and geologic fluids are needed for resource recovery and contaminant assessment and monitoring.

– New and more sensitive isotopic tracer methods will contribute to evaluation of natural and anthropogenic processes in the geologic environment.

– Improved understanding of hydrologic processes, especially focusing on scaling and heterogeneity of porosity and permeability distributions will form the basis for more robust predictions of flow in reservoirs, aquifers, or in unconfined groundwater.

– Rock physics and geomechanics studies form the foundation for improved geophysical imaging, and for understanding fracture-mediated subsurface transport of fluids.

- *Environmental Sciences:* Within the Office of Biological and Environmental Research, there are research programs on global climate change, advanced sensors, and integrated assessment of the impacts of climate change.

- *Computational Sciences:* Within the Office of Computational and Technology Research, efforts at improving computational tools, developing the 2nd generation Internet, and providing the basis for massively parallel computation are critical to enhancing domestic supplies.

It is worth noting that beyond SC's contributing basic science, the Office of Environmental Management and the Office of Defense Programs both conduct basic research that impacts domestic supplies. The Office of Environmental Management conducts research that provides a sound scientific basis for assessing risks of various supply technologies. And, Defense Programs supports research in computing technology, computational modeling, instrumentation development, and geophysical studies that have both defense and civilian applications.

Producing Clean Fuels

Examples of basic science that support Producing Clean Fuels are provided below. Most of this research is carried out by the Office of Basic Energy Sciences and the Office of Biological and Environmental Research.

Efforts to develop cleaner fuels and reduce carbon emissions draw on many scientific disciplines. For example: biochemistry; catalysis; molecular, cellular and plant biology; structural biology; genome science; and solar photochemistry contribute, because the production of fuels and chemicals by plants and microorganisms and the interconversion of greenhouse gases requires a better understanding of metabolism, of the structure and function of sub-cellular components, and of enzymes. Similarly, the state-of-the-art in biochemistry, molecular biology, and ecology contribute. All of these biological processes are important in understanding the role of microorganisms in sequestering carbon. Improvements in combustion to reduce carbon emissions require a fundamental understanding in chemical dynamics, theoretical chemistry, and physics. Conversion of sunlight to energy requires an understanding in many areas of science, including photochemistry, photosynthesis, metabolism, and solid-state physics. The search for increased efficiency in energy production and use requires fundamental knowledge in ceramics, metals, polymers, solid-state chemistry, and condensed matter physics for materials that can withstand higher temperatures, have lower coefficients of friction, and are stronger and lighter. Enhanced recovery of fuel resources and of disposal of carbon dioxide requires a fundamental understanding of geometric, structural, and hydrologic properties of reservoirs and of multiphase, nonlinear transport of fluids in porous and fractured structures. Cross-cutting programs in nano- and meso-phase materials involve research at the forefront of materials science, chemistry, engineering, surface science, and semiconductor physics.

Office of Science fundamental research areas that underpin the Clean Fuels R&D Portfolio—and other DOE science and technology portfolios—include the following.

- *Microbial Genome Program:* Significant investments have been made in the technology that enables genome sequencing at rates previously unattainable. Capitalizing on these investments, the genomes of microbes that produce methane and hydrogen will be sequenced. This will enable the identification of the key genetic components of the organisms that regulate these gases. Once we identify and understand more fully how the enzymes and organisms operate, we will be able to evaluate the potential use of either the microorganisms or the relevant enzymes to produce methane or hydrogen from either fossil fuels or other carbonaceous sources, including biomass or perhaps even some kinds of waste products. For instance, recently discovered "extremophile" organisms could be used to engineer biological entities that could ingest a feedstock like methane, sequester the carbon dioxide, and give off hydrogen.

- *Microbial Conversion*: Basic research in microbial conversion focuses on examining the metabolism, biochemistry, genetics, and physiology of organisms and consortia of organisms that degrade lignin, cellulose, and/or hemicellulose into potential fuels. The fuels include ethanol, higher alcohols, and methane. While much of the activities involve anaerobic bacteria, fungi are also actively investigated. These studies form the foundation for the efficient conversion of lignocellulosics (biomass) into potential liquid and gaseous fuels, an important component of several technology programs in this portfolio.

- *Plant Biology*: Green plants and some bacteria use photosynthesis to capture solar energy and convert it into chemical energy that fuels metabolism and the biosynthesis of a broad range of storage compounds and structural components. For example, the chemical energy in firewood was the early energy source for mankind, and even today the worldwide combustion of plant biomass generates more energy than any other non-fossil fuel source. As a renewable resource, plant biomass potentially has enormously valuable uses when it is converted into specific materials, fuels, chemical feedstocks and petroleum replacing materials. Basic studies in plant biology are providing new insights into the genetic, metabolic, and enzymatic properties of plants that regulate the production of specific useful chemical compounds and materials. Similarly, studies on the regulation of the photosynthetic process that fuels metabolic biosynthesis are yielding new insights on how bacteria and plants channel photosynthetic energy into the production of renewable biomass materials.

- *Solar Photochemistry:* This research explores fundamental photochemical processes aimed at the capture and conversion of solar energy. This research program encompasses organic and inorganic photochemistry, electron and energy transfer in homogeneous and heterogeneous media, photocatalysis, and photoelectrochemistry. The photosynthetic reaction center is studied as a model for the design of efficient, photoinduced charge separation in biomimetic/ photocatalytic assemblies. The research provides the foundations for future solar technologies in which light-induced, charge-separation processes will convert light energy to chemical energy in such applications as the production of alcohols from carbon dioxide, hydrogen from water, or ammonia from atmospheric nitrogen.

- *Catalysis:* Catalysis is a chemical process found widely in nature and used extensively in industry because it removes energy barriers to chemical reactions. Catalysts used for the refining of petroleum or the manufacture of chemicals are important because they reduce process energy, speed up production, and make possible the manufacture of new materials. Despite their importance, catalytic processes are not sufficiently well understood to allow for rational design of new catalysts. Models for catalytic action are limited in scope and applicability. The Office of Science catalysis program seeks to gain understanding of catalysis at the molecular level to allow the development of general theories and models of catalytic action. The program includes both heterogeneous (multiple phases such as liquid/solid) and homogeneous (single phase) catalysis. Research in heterogeneous catalysis seeks to characterize the role of surface properties on molecular transformations and the structural relationships between oxide surfaces and reaction pathways, especially in the acid and redox catalysts commonly encountered in industrial applications. Research in homogeneous catalysis seeks to characterize the activation and subsequent reactions of carbon-hydrogen bonds and the role of bonding and molecular structure on the catalytic processes. The program constitutes the largest single component of the Nation’s basic research portfolio focused on chemical catalysis.

The Department of Energy's Climate Change Technology Initiative has been developed as a partnership between the technology and research offices at DOE and representatives of the National Laboratories. A series of workshops have been held to identify basic science needs and opportunities for capturing and sequestering carbon, for fuel cell and hydrogen development, for enhancing the natural carbon cycle, and for biomass conversion. These workshops have included participants from the Offices of Science, Fossil Energy, and Energy Efficiency and Renewable Energy.

Advanced Power Systems

Examples of basic science that support Advanced Power Systems are provided below. Most of this research is carried out by the Office of Basic Energy Sciences, the Office of Biological and Environmental Research, and the Office of Fusion Energy Sciences.

Efforts to develop clean power and reduce carbon emissions draw on many scientific disciplines. For example: electrochemistry; combustion; materials - including welding, joining, and corrosion; photovoltaics and semiconductors; engineering research; geosciences; biology and genomics; and environmental sciences. These and other disciplines contribute, because power production, transmission, and storage as well as the interconversion of greenhouse gases requires a better understanding of the materials and processes that contribute to each phase. Similarly, the state-of-the-art in biochemistry, molecular biology, and ecology will be impacted. All of these biological processes are important, for example, in understanding the role of marine microorganisms in sequestering carbon. Improvements in combustion to reduce carbon emissions require a fundamental understanding in chemical dynamics and theoretical chemistry and physics. The search for increased efficiency in energy production and use requires fundamental knowledge in ceramics, metals, polymers, solid-state chemistry, and condensed matter physics for materials that can withstand higher temperatures, have lower coefficients of friction, and are stronger and lighter. Enhanced recovery of fuel resources, the disposition of nuclear power and other transuranic waste, and the disposal of carbon dioxide require a fundamental understanding of geometric, structural, and hydrologic properties of reservoirs and of multi-phase, nonlinear transport of fluids in porous and fractured structures. Cross-cutting programs in nano- and meso-phase materials involve research at the forefront of materials science, chemistry, engineering, surface science, and semiconductor physics. And efforts to understand fusion plasma science and concepts for engineering plasma confinement may someday make commercial nuclear fusion a reality.

Contributions to Advanced Power Systems include the following research areas:

- *Electrochemistry:* Fundamental research is supported in areas critical to understanding the underlying limitations in the performance of non-automotive electrochemical energy storage systems. Areas of research include the characterization of anode, cathode, and electrolyte systems and their interactions. The broad spectrum of research includes fundamental studies of composite electrode structures, failure and degradation of active electrode materials, and thin film electrodes, electrolytes, and interfaces. The aim is providing knowledge that will lead to improvements in battery size, weight, life, and recharge cycles.

- *Combustion:* Basic research in combustion provides knowledge on the rates and energetics of chemical reactions and on the interactions of fluid dynamics and chemistry. This knowledge is required by combustion models used for the design and optimization of energy-efficient, reduced-emission combustion devices. Knowledge gained consists of measured properties as well as theoretical constructs for the reliable prediction or extrapolation of such properties. SC supports the operation of the Combustion Research

Facility (CRF) at Sandia National Laboratories, California, where collocated research, supported by SC, the Office of Energy Efficiency and Renewable Energy (EE), the Office of Fossil Energy (FE), and industry, is conducted in a highly collaborative environment.

- *Photovoltaics and Semiconductors:* Semiconducting materials underpin virtually the entire "high tech" industry worldwide. They comprise the building blocks and components for several technologies within this portfolio, including photovoltaics, sensors, power electronics, and high speed computational systems. Research within this area includes synthesis of new and tailored semiconductor materials; characterization of structure, electronic structure, and stability of semiconductors; investigations of surfaces and interfaces; the influence of light on the behavior and properties of semiconductor materials; theory and modeling of properties and behavior; and the operation of facilities that support such research.

- *Ceramic Materials:* Ceramic materials play an integral role in the utility, automotive, and other energy-intensive industries. A fundamental understanding of their complex microstructure and behavior is essential for their successful implementation. The ceramic sciences research addresses the scientific issues underlying the synthesis, processing, behavior, and characterization of ceramic and non-metallic glassy materials. Focus areas include synthesis, processing, reactivity, and physical and mechanical properties, with emphasis on elevated temperature behavior. The technological areas impacted include high temperature structural materials (e.g., high temperature monolithic and composite ceramics and ceramic coatings), energy storage materials (e.g., solid electrolytes, batteries, and ultracapacitors), energy conversion materials (e.g., fuel cells), hazardous waste storage materials (glasses and ceramics), sensors, and environmentally benign synthesis techniques.

- *Radiation Materials:* There are approximately 70 nuclear power reactors in the United States that are over 20 years old. The time-dependent radiation-induced embrittlement of aging steel containment vessels and structural members defines a critical safety and environmental problem for these on-line facilities. Their continued safe operation requires a better predictive "early warning" or "retirement for cause" model for their behavior. Therefore, the Office of Science supported research in radiation materials includes synergistic relationships between neutron, proton, and ion irradiation with defects, composition, and physical and mechanical behaviors in metals, ceramics, intermetallics, polymers, and semiconductors. Emphasis is on surface modification, modeling of radiation induced damage, cascade formation, property changes, design of radiation-resistant materials, irradiation induced stress-corrosion cracking, changes in grain boundary microchemistry, crack tip phenomena, and evaluation of spallation neutron and high energy proton damage. There are three additional distinct motivations for SC activities in radiation materials sciences: (1) the safe containment, over many-generations, of radioactive wastes requires valid predictive models for their time-dependent degradation under conditions including self-irradiation, heat, and the time-dependent production of radio-decay products (this work supports the Department's efforts in Environmental Management); (2) the development of fusion reactors will require an understanding and a modeling of the radiation induced behavior of insulator and first wall component candidate materials such as silicon carbide, high-chromium ferritic-martensitic steels, and vanadium; and (3) the energetic-ion-induced surface modification and implantation of metals, ceramics, polymers, and semiconductors is a continuously evolving science as well as an important technology that in turn underpins all energy conversion and conservation technologies.

- *High Temperature Superconducting Materials:* Research into the development of improved superconductors that can be used in the generation, transmission, utilization, and storage of electric power using high-T_c superconductors contributes to the efficient utilization of energy. Therefore, basic research is performed on the theory, synthesis, processing, structure, and physical properties of high temperature superconducting materials including the discovery of new classes of superconducting materials.

- *Intermetallics:* Intermetallic compounds are metal to metal compounds with definite stoichiometry. Intermetallic alloys made from these compounds constitute a unique class of high-temperature structural materials that posses the desired properties of high strength, oxidation and corrosion resistance, low density, and a high melting point. Such properties make them attractive as constituents for gas turbine engines, high-temperature coatings, and in dies and molds for ceramic and metallurgical processing. Intermetallic compounds may also be used in a variety of electromagnetic areas including both hard and soft magnets, superconductor, semiconductor, and optical applications.

- *Materials Welding and Joining:* Materials welding and joining are critical fabrication technologies that are used extensively in all energy, automotive, environmental, and electronic technologies. Weld failures are the most frequent reason for unscheduled and sometimes catastrophic outages in power plants with the cost of replacement power often exceeding $1 million dollars per day. Welding represents 10 percent of the cost of construction and 20 percent of the maintenance costs for a 500 megawatt fossil-fueled electric power plant. SC supported basic research includes understanding the microstructure and defects that develop as a consequence of temperature gradients; solid-state phase transformations in weld heat affected zones; thermal processes as applied to gas metal arc welding; molten metal droplet formation; plasma and arc physics; laser welding of automotive aluminum alloys; time-resolved X-ray absorption spectroscopy to directly determine rate of transformation of one phase to another phase under the highly-nonisothermal conditions that prevail during welding; welding of Al, Ti, and thin plates; coupling welding science and fracture mechanics modeling in response to the Northridge California earthquake experience; and critical issues in the non-welding joining of ceramics and dissimilar materials.

- *Corrosion:* The importance of the scientific understanding of corrosion is emphasized by the estimate that corrosion in the United States has an economic cost of 4 percent of the gross domestic product. Corrosion damage limits the performance of all energy conversion technologies. The basic research underlying the science of corrosion focuses on the formation, properties, and breakdown of passivating films; on a wide array of electrochemical phenomena involved in aqueous corrosion such as pitting and crevice corrosion; on high-temperature gaseous corrosion; and on new techniques to identify and study corrosion.

- *Engineering Research:* The SC Engineering Program supports fundamental research on broad, generic topics in energy related engineering topics. This includes research on fractals and porous media transport, nonlinear waves, traveling wave convection in fluid mixtures, wave turbulence interactions, multi-phase systems, gas and solids problems, the effect of different Reynolds numbers on turbulence, mixing and transport, gas-liquid flow in pipelines, lubricated transport of viscous materials, the rheology of concentrated suspensions, macrostatistical hydrodynamics, heat/mass transfer enhancement in separated and vortex flows, effect of forced and natural convection on solidification of binary mixtures, interfacial area and transfer in two-phase flow, and various diagnostics for analyzing fluids. An emphasis of the research is on complicated fluid dynamics because fluids are a part of most energy-related systems including pipelines, manufacturing processing, hydraulic systems, planes, trains, automobiles, ships, liquid metal handling, new materials synthesis, chaotic wave motion, weather prediction, environmental issues, and biological systems.

- *Geosciences:* Both geophysical and geochemical information is significant for current and future energy technologies, particularly geothermal energy, oil and gas, and understanding the disposition of wastes generated by the technological enterprise, including the by-products of nuclear energy. Rock mechanics, fracture, and fluid flow encompasses research on the response of rock to stress and the role of fluid flow as a cause and/or effect. The prediction and interpretation of rock response offers unique challenges because the scales involved range from the microscopic to hundreds of kilometers and from seconds to geologic times. The properties of rock are dominated by extreme heterogeneity, pressure dependence, the presence of natural fracture systems, and the coupling between thermomechanical properties, fluid flow, and geochemical processes. Geochemical research is supported in rock-fluid interactions to provide fundamental information on the governing mechanisms and rates of reactive geochemical processes that concentrate, transport, modify, and emplace energy resources and the by-products of energy use within the Earth's shallow crust. Other research in the Geosciences is focused on gaining a better understanding of the fundamental biological, chemical, geological, and physical processes that must be marshalled for the development and advancement of new, effective, and efficient processes for the remediation and restoration of contaminated sites. Research advances will continue to be made from pore to field scales, on genes and proteins used in bioremediation, in non-destructive, real-time measurement techniques, in overcoming physico-chemical impediments to bacterial mobility in the subsurface, on species interaction and response of microbial ecology to contamination, and in understanding microbial processes for altering the chemical state of metallic and radionuclide contaminants.

- *Fusion Energy Sciences:* Research is focused on fusion plasma science and engineering concepts and supporting science for plasma confinement. SC maintains a large research program aimed at unlocking the secrets to this potentially limitless supply of clean energy. Supporting computational sciences are developed within the Office of Computational and Technology Research. Materials and superconductivity research are critical to various confinement concepts.

- *Biology/Genomics:* The microbial genome program capitalizes on DNA sequencing technology from the human genome program to determine the complete DNA sequence of microbes with potential environmental, energy, or commercial applications. While the program has a principal emphasis on DNA sequencing it includes research on microbial diversity, to identify a broader array of potentially useful microbes; and novel strategies and tools for characterizing, manipulating, and modeling entire reaction pathways or regulatory networks of microbes or groups of microbes to maximize the usefulness of these newly characterized microbes.

- *Structural Biology:* Understanding and predicting the complex relationship between the DNA sequence of a gene and the structure and function of the protein it encodes is a critical first step in being able to reengineer genes and proteins for use in developing new strategies for improving or developing new fuels, reducing pollution from fuel use, and cleaning up the environment. Therefore, SC supports basic research in structural biology including instrumentation research and research that cuts across basic, molecular, and computational biology. For example, studies of inverse protein folding provide an understanding of the rules that proteins follow to acquire the three dimensional structures that give them their biological function while Proteomics research provides information that will lead to an understanding of the structure, function, and interactions of all proteins encoded by an organism's genome.

- *Environmental Sciences:* Research in the environmental sciences is focused on understanding the basic chemical, physical, and biological processes of the Earth's atmosphere, land, and oceans and how these processes may be affected by energy production and use, primarily the emission of carbon dioxide from fossil fuel combustion. A major part of the research is designed to provide the data that will enable an objective assessment of the potential for, and consequences of, global warming. Emphasis is given to understanding the radiation balance from the surface of the Earth to the top of the atmosphere (including the role of clouds) and on enhancing the quantitative models necessary to predict possible climate change at global and regional scales. The Atmospheric Radiation Measurement (ARM) program works to produce the experimental and modeling results that will be necessary to resolve the greatest uncertainty in climate prediction—the role of clouds and solar radiation. Climate modeling using massively-parallel supercomputers will simulate climate change, predict climate, and evaluate model uncertainties due to changes in atmospheric concentrations of greenhouse gases on decade to century time scales. The Carbon Cycle program studies the natural carbon cycle and assesses the potential impacts of climate change on terrestrial systems.

  Unique facilities at the Environmental Molecular Sciences Laboratory such as the Molecular Science Computing Facility, the High-Field Mass Spectrometry Facility, and the High-Field Magnetic Resonance Facility will be used to conduct a wide variety of molecular-level environmental science research, including movement of contaminants in subsurface groundwater and vadose zone sediments and atmospheric chemical reactions that contribute to global warming.

Capitalizing on activities in support of the U.S. Global Change Research Program, and stimulating a partnership between the technology and research offices at DOE and representatives of the National Laboratories, the Climate Change Technology Initiative supports research into the role that the terrestrial biosphere and human activities play on the state and quality of the global climate. The research seeks the understanding necessary to exploit the biosphere's natural processes for use in sequestration of atmospheric carbon dioxide including the roles of marine microorganisms in ocean carbon sequestration and the mechanisms by which forest ecosystems sequester carbon. A series of workshops have been held to identify the basic science needs and opportunities for capturing and sequestering carbon, for fuel cell and hydrogen development, for enhancing the natural carbon cycle, and for biomass conversion. These workshops have included participants from the Offices of Science, Fossil Energy, and Energy Efficiency and Renewable Energy.

In addition to interactions across the Department to develop the Climate Change Technology Initiative, the SC programs maintain significant interactions with other DOE offices and other agencies involved in environmental remediation, e.g., Office of Environmental Management, the Environmental Protection Agency, the Department of Defense, or other partners in the U.S. Global Change Research program.

Enhancing Utility Infrastructure

Examples of basic science that support Utility Infrastructure are provided below. Most of this research is carried out by the Office of Computational and Technology Research and the Office of Basic Energy Sciences.

- *Advanced Computing:* High speed computing and networking capabilities are critical to both modeling and control of the utility infrastructure.

- *Materials Science and Physics:* A wide range of advanced materials and materials processing technologies are required for high-performance low-cost semiconductors, superconductors, high-strength light-weight composites, and corrosion resistant materials. Physical understanding of the properties of these materials aids researchers in improving performance and reducing cost.

- *Power Electronics and Controls:* Research includes the development of advanced topology modeling methodologies and high speed switching devices based on silicon carbide and thin-film diamond which will have higher capacity, lower cost and lower losses.

- *Energy Storage:* Research in this area addresses advanced batteries, supercapacitors, flywheel technologies and their associated materials, and control technologies.

The performance parameters, economics, environmental acceptability and safety of all energy generation, conversion, transmission, and conservation technologies are limited by the performance of available materials. The BES Materials Sciences Program is concerned with understanding and exploiting the synergistic relationship between the synthesis, processing, structure, properties, behavior, in-service performance and lifetime, and recyclability of materials. Such understanding is necessary for the development of technologically and economically desirable new materials and cost-competitive and environmentally acceptable methods for their synthesis, processing, fabrication, quality manufacture, and recycling. The Materials Sciences program funds basic research in metallic glasses (for corrosion resistant, wear resistant, and low magnetic loss behavior); ceramics (energy storage technologies); high temperature superconductivity (for energy generation, transmission, and storage); hard and soft magnets (for low energy loss motors and transformers); and ordered intermetallic alloys (for heat, load, wear, and corrosion resistant applications).

Within the BES Chemical Sciences Program, the Advanced Battery Research program supports fundamental research in areas critical to understanding the underlying limitations in the performance of non-automotive electrochemical energy storage systems. Areas of research include anode, cathode, and electrolyte systems and their interactions with emphasis on improvements in battery size, weight, life, and recharge cycles. Although both primary and secondary battery systems are considered, the greatest emphasis is placed on rechargeable (i.e., secondary) battery systems. The program covers a broad spectrum of research including fundamental studies of composite electrode structures, failure and degradation of active electrode materials, and thin film electrodes, electrolytes, and interfaces. Problems of electrode morphology, corrosion, electrolyte stability, and the transport properties of electrode and electrolyte materials and surface films are also addressed.

In Superconductivity research particularly, the Office of Basic Energy Sciences (BES) plays a significant role. It funds research at the Oak Ridge National Laboratory (ORNL) to work with the 3M Company and develop a novel *ex situ* process for growing superconducting films. This work is conducted in collaboration with the Office of Energy Efficiency and Renewable Energy (EE) Second Generation Wire Initiative. The project included BES funding of $375,000 over 18 months, with a matching amount at ORNL from EE. Over the 18 month project time frame, 3M Company devoted over $1.5 million to research with both ORNL and Los Alamos National Laboratory (LANL) on aspects of the second generation wire initiative. EE and SC superconductivity research is coordinated through several workshop mechanisms, including a Wire Workshop jointly sponsored by EE/SC. The output is a jointly produced, publicly available document describing key science issues identified at the workshop. Teams of EE/BES staff have also been formed to focus on specific issues. In addition, SC maintains facilities on which advanced energy research can be carried out and a large communication network and computer facilities where information can be shared and simulations and analysis can be done.

Clean and Efficient Vehicles

Examples of basic science that support Clean and Efficient Vehicles are provided below. Most of this research is carried out by the Office of Basic Energy Sciences (BES).

- *Electrochemistry:* Within this topic area, the BES Advanced Battery Research program supports basic research critical to understanding limitations in the performance of electrochemical energy storage systems. Research addresses the characterization of anode, cathode, and electrolyte systems and their interactions, and includes fundamental studies of composite electrode structures, failure and degradation of electrode materials, and thin film electrodes, electrolytes, and interfaces. Close coordination with DOE's Office of Transportation Technologies' (OTT) battery programs is accomplished through joint meetings, program reviews, and strategy sessions.

- *Combustion:* Basic research in combustion provides knowledge on the rates and energetics of chemical reactions and on the interactions of fluid dynamics and chemistry. This knowledge is required by combustion models used for the design and optimization of energy efficient, low emission combustion devices. BES supports the operation of the Combustion Research facility at Sandia National Laboratory, which serves as the focus for the integration with the applied combustion programs in EE. Additionally, the EE Combustion Cooperative Research and Development Agreement (CRADA) is one of two pilot collaboratory projects in the Office of Science sponsored DOE 2000 Initiative.

- *Synthesis and Processing of Advanced Materials:* These essential elements of materials science and engineering deal with the assembly of atoms or molecules to form materials, the manipulation and control of the structure at all levels from the atomic to the macroscopic scale, and the development of processes to produce materials for specific applications. The goal of the basic research ranges from creating new materials, improving the properties of known materials, and improving the forming of metals to the understanding of such phenomena as diffusion, crystal growth, sintering, and phase transitions. Scientific results are translated into useful materials by developing processes capable of producing high quality cost-effective products including light weight alloys for vehicles.

- *Ceramics:* The BES Ceramics program addresses scientific issues related to the synthesis, processing, and characterization of ceramic and non-metallic glassy materials. The OTT technological areas impacted include high temperature structural materials (ceramic coatings), energy storage materials (batteries), energy conversion materials (fuel cells), and sensors.

- *Semiconductors:* This research includes synthesis and characterization of new semiconductor materials, electronic structure and stability studies, investigations of surfaces and interfaces, the influence of light on semiconductor properties, and theory and modeling. Semiconductors are the building blocks for photovoltaics, sensors, power electronics, and high speed computational systems.

- *Welding and Joining Sciences:* Welding and joining are critical fabrication technologies used in the automotive industry. BES research includes studies to understand the microstructure and defects that develop due to temperature gradients, solid-state phase transformations in weld heat affected zones, thermal processes as applied to gas metal arc welding, molten metal droplet formation, plasma and arc physics, laser welding of aluminum alloys, and joining of ceramics and dissimilar materials. These activities are directly related to the Transportation Materials program in OTT.

Many of the OTT/BES integration activities, especially those addressing materials research and development, occur through the Energy Materials Coordinating Committee (EMaCC).

Efficient and Affordable Buildings

Examples of basic science that support Efficient and Affordable Buildings are provided below. Most of this research is carried out by the Office of Basic Energy Sciences.

- *Electrochemistry:* Fundamental research is supported in areas critical to understanding the underlying limitations in the performance of non-automotive electrochemical energy storage systems. Areas of research include the characterization of anode, cathode, and electrolyte systems and their interactions. The broad spectrum of research includes fundamental studies of composite electrode structures, failure and degradation of active electrode materials, and thin film electrodes, electrolytes, and interfaces.

- *Combustion:* Basic research in combustion provides knowledge on the rates and energetics of chemical reactions and on the interactions of fluid dynamics and chemistry. This knowledge is required by combustion models used for the design and optimization of energy-efficient, reduced-emission combustion devices. Knowledge gained consists of measured properties as well as theoretical constructs for the reliable prediction or extrapolation of such properties. BES supports the operation of the Combustion Research Facility (CRF) at Sandia National Laboratories, California, where collocated research, supported by BES, the Office of Energy Efficiency and Renewable Energy, the Office of Fossil Energy, and industry, is conducted in a highly collaborative environment.

- *Ceramic Materials:* Ceramic materials play an integral role in the utility, automotive, and other energy-intensive industries such as the building industry. A fundamental understanding of ceramic materials' complex microstructure and behavior is essential for their successful implementation. BES research addresses the scientific issues underlying the synthesis, processing, behavior, and characterization of ceramic and non-metallic glassy materials. The technological areas impacted include high temperature structural materials (e.g., high temperature monolithic and composite ceramics and ceramic coatings), energy storage materials (e.g., solid electrolytes, batteries, ultracapacitors), and energy conversion materials (e.g., fuel cells), sensors, and environmentally benign synthesis techniques.

- *Semiconductors:* Semiconducting materials underpin virtually the entire "high tech" industry worldwide. They comprise the building blocks and components for several technologies within this portfolio, including photovoltaics, sensors, power electronics, and high speed computational systems. Research within this area includes synthesis of new and tailored semiconductor materials; characterization of structure, electronic structure, and stability of semiconductors; investigations of surfaces and interfaces; the influence of light on the behavior and properties of semiconductor materials; theory and modeling of properties and behavior; and the operation of facilities that support such research.

Clean and Productive Industries

Examples of basic science that support Clean and Productive Industries are provided below. Most of this research is carried out by the Office of Basic Energy Sciences and the Office of Computational and Technology Research.

- *Combustion:* Basic research in combustion provides knowledge on the rates and energetics of chemical reactions and on the interactions of fluid dynamics and chemistry. This knowledge is required by combustion models used for the design and optimization of energy-efficient, reduced-emission combustion devices for most industrial processes. Knowledge gained consists of measured properties as well as theoretical constructs for the reliable prediction or extrapolation of such properties. The Office of Basic Energy Sciences supports the operation of the Combustion Research Facility (CRF) at Sandia National Laboratories, California, where collocated research, supported by SC, the Office of Energy Efficiency and Renewable Energy, the Office of Fossil Energy, and industry, is conducted in a highly collaborative environment.

- *Catalysis:* Catalysis is a chemical process found widely in nature and used extensively in industry because it removes energy barriers to chemical reactions. Catalysts used for the refining of petroleum or the manufacture of chemicals are important because they reduce process energy, speed up production, and make possible the manufacture of new materials. Despite their importance, catalytic processes are not sufficiently understood to allow for rational design of new catalysts. Models for catalytic action are limited in scope and applicability. The SC catalysis program seeks to gain understanding of catalysis at the molecular level to allow the development of general theories and models of catalytic action. The program includes both heterogeneous (multiple phases such as liquid/solid) and homogeneous (single phase) catalysis. Research in heterogeneous catalysis seeks to characterize the role of surface properties on molecular transformations and the structural relationships between oxide surfaces and reaction pathways, especially in the acid and redox catalysts commonly encountered in industrial applications. Research in homogeneous catalysis seeks to characterize the activation and subsequent reactions of carbon-hydrogen bonds and the role of bonding and molecular structure on the catalytic processes. The program constitutes the largest single component of the Nation's basic research portfolio focused on chemical catalysis.

- *Synthesis and Processing of Advanced Materials:* These essential elements of materials science and engineering deal with the assembly of atoms or molecules to form materials, the manipulation and control of the structure at all levels from the atomic to the macroscopic scale, and the development of processes to produce materials for specific applications. The goal of the basic research ranges from creating new materials, improving the properties of known materials, and improving the forming of metals to the understanding of such phenomena as diffusion, crystal growth, sintering, and phase transitions. Scientific results are translated into useful materials by developing processes capable of producing high quality cost-effective products including light weight alloys for vehicles.

- *Ceramics:* Ceramic materials play an integral role in the utility, automotive, and other energy-intensive industries. A fundamental understanding of their complex microstructure and behavior is essential for their successful implementation. BES ceramic sciences research addresses the scientific issues underlying the synthesis, processing, behavior, and characterization of ceramic and non-metallic glassy materials. Focus areas include synthesis, processing, reactivity, and physical and mechanical properties, with emphasis on elevated temperature behavior. The technological areas impacted include high temperature structural materials (e.g., high temperature monolithic and composite ceramics and ceramic coatings), energy storage materials (e.g., solid electrolytes, batteries, ultracapacitors), sensors, and environmentally benign synthesis techniques.

- *Intermetallics*: These are metal to metal compounds with definite stoichiometry. Intermetallic alloys made from these compounds constitute a unique class of high-temperature structural materials that posses the desired properties of high strength, oxidation and corrosion resistance, low density, and a high melting point. Such properties make them attractive as constituents for high-temperature coatings and in dies and molds for ceramic and metallurgical processing.

- *Welding and Joining Sciences:* Welding and joining are critical fabrication technologies used in the automotive industry. BES research includes studies to understand the microstructure and defects that develop due to temperature gradients, solid-state phase transformations in weld heat affected zones, thermal processes as applied to gas metal arc welding, molten metal droplet formation, plasma and arc physics, laser welding of aluminum alloys, and joining of ceramics and dissimilar materials.

- *Corrosion:* The importance of the scientific understanding of corrosion is emphasized by the estimate that corrosion in the United States has an economic cost of 4 percent of the gross domestic product. Corrosion damage limits the performance of industrial processes. The basic research underlying the science of corrosion focuses on the formation, properties, and breakdown of passivating films on a wide array of electrochemical phenomena involved in aqueous corrosion such as pitting and crevice corrosion, on high-temperature gaseous corrosion, and on new techniques to identify and study corrosion.

- *Engineering Research:* The BES Engineering Program supports fundamental research on broad, generic topics in energy related engineering topics. An emphasis of the research is on complicated fluid dynamics because fluids are a part of most energy-related systems and industrial processes, including pipelines, manufacturing processing, hydraulic systems, liquid metal handling, new materials synthesis, chaotic wave motion, environmental issues, and biological systems. Engineering topics include fractals and porous media transport, nonlinear waves, traveling wave convection in fluid mixtures, wave turbulence interactions, multi-phase systems, gas and solids problems, the effect of different Reynolds numbers on turbulence, mixing and transport, gas-liquid flow in pipelines, lubricated transport of viscous materials, the rheology of concentrated suspensions, macrostatistical hydrodynamics, heat/mass transfer enhancement in separated and vortex flows, effect of forced and natural convection on solidification of binary mixtures, interfacial area and transfer in two-phase flow, and various diagnostics for analyzing fluids.

- *Plant Sciences:* Green plants and some bacteria use photosynthesis to capture solar energy and convert it into chemical energy that fuels metabolism and the biosynthesis of a broad range of storage compounds and structural components. For example, the chemical energy in firewood was the early energy source for mankind, and even today the worldwide combustion of plant biomass generates more energy than any other non-fossil fuel source. As a renewable resource, plant biomass potentially has enormously valuable uses when it is converted into specific materials, fuels, chemical feedstocks, and petroleum replacing materials. Basic studies in plant biology are providing new insights into the genetic, metabolic, and enzymatic properties of plants that regulate the production of specific useful chemical compounds and materials. Similarly, studies on the regulation of the photosynthetic process that fuels metabolic biosynthesis are yielding new insights on how bacteria and plants channel photosynthetic energy into the production of renewable biomass materials.

- *Biology/genomics:* The microbial genome program capitalizes on DNA sequencing technology from the human genome program to determine the complete DNA sequence of microbes with potential environmental, energy, or commercial applications. While the program has a principal emphasis on DNA sequencing, it includes research on microbial diversity, to identify a broader array of potentially useful microbes; and novel strategies and tools for characterizing, manipulating, and modeling entire reaction pathways or regulatory networks of microbes or groups of microbes to maximize the usefulness of these newly characterized microbes.

- *Structural Biology:* Understanding and predicting the complex relationship between the DNA sequence of a gene and the structure and function of the protein it encodes is a critical first step in being able to reengineer genes and proteins for use in developing new strategies for improving or developing new fuels, reducing pollution from fuel use, and cleaning up the environment. Therefore, the Office of Science supports basic research in structural biology including instrumentation research and research that cuts across basic, molecular, and computational biology. For example, studies of inverse protein folding provide an understanding of the rules that proteins follow to acquire the three dimensional structures that give them their biological function, while Proteomics research provides information that will lead to an understanding of the structure, function, and interactions of all proteins encoded by an organism's genome.

- *Computational Sciences:* The computational research area provides tools and methods to enable the wide spread use of massively parallel computers and the high speed network connections which underpin the computational needs common to many of the industry vision statements and their need for advanced computational capability for industry process understanding and control.

- *Chemical Sciences:* Research in chemistry focuses on fundamental molecular level understanding of chemical interactions and chemical reactions that provide the basis for new analytical tools and methods and the physical and chemical interactions that support the development of new membranes for separation processes.

- *Materials Science:* Basic research in materials enables technologies underpinning new aluminum alloys, the high rate sheet metal forming of aluminum alloys, and high strength and corrosion resistant intermetallic alloys. Part of this effort is carried out under the Design and Synthesis of Ultrahigh-Temperature Intermetallics project under the distributed DOE Center of Excellence for the Synthesis and Processing of Advanced Materials (CSP). Research is also underway, coordinated and carried out under the Materials Joining project under CSP, on the reliable joining of materials both for on-line repair and for the fabrication of new systems encompassing both metals and ceramics. Additional research involves efforts to advance materials requiring long-lifetime wear resistant surfaces, for example, to form boron nitride and diamond protective films on materials and investigating and understanding how to form oxide films as protective layers to prevent corrosion.

- *Advanced Sensors:* Research is conducted on innovative, more powerful sensors, including the understanding of the chemistry of molecular interactions that generate a chemical or physical response.

- *Computation:* The computational research area provides tools and methods to enable the widespread use of massively parallel computers and the high speed network connections which underpin the computational needs common to many of the industry vision statements and their need for advanced computational capability for industry process understanding and control.

Science Excellence and Research Integration

Recognizing that the basic sciences are the cornerstone for future technology innovation, it is important that DOE's basic science be well integrated with applied technology programs and that research be of the highest caliber. At the same time, consideration of needs and applications does not and should not constrain the scope of scientific inquiry—this is the hallmark of a basic science program and a fundamental tenet for truly crosscutting scientific discovery and innovation.

Consistent with the goal for science excellence, SC implements a highly effective scientific peer review process and is often called upon to conduct peer review for the rest of the Department. Additionally, and over the last few years, the Office of Science has strengthened its process for integration with the applied energy R&D programs, improving coordination and communication across a broad range of areas. Examples of some specific energy technology areas that have benefitted from recent strengthened integration include:

- Office of Energy Efficiency and Renewable Energy's Industries of the Future Program.
- Partnership for a New Generation Vehicle.
- Advanced Computation Initiative, that includes the Office of Energy Efficiency and Renewable Energy as well as the oil and gas industry.
- Advanced Turbine Systems Program.

Thus, with an eye toward research relevance and integration, SC sets strategic research directions through working relationships with other DOE programs, through research workshops involving input from the scientific and technical communities, through the promotion of open information transfer and exchange of ideas between the basic and applied research communities, and, finally, through the sponsorship of selected high-impact research collaborations and partnerships. Individual research projects are funded based on peer review by the members of the scientific community. These approaches to basic research funding have led to hundreds of Cooperative Research and Development Agreements, that extend the basic research to applications and development. In addition, there are many more collaborations between SC researchers and industrial researchers.

The resulting diverse portfolio of basic research programs and the combination of university and laboratory programs supports the institutional capacity for interdisciplinary research needed to solve the problems of energy production and use, and also integrates basic science with applied science and development activities. The Department's National Laboratory system plays a special role in the ability of SC to effectively integrate research and development by providing opportunities to collocate activities at these sites. And, because many researchers are also cofunded by SC as well as the applied energy technology programs, the Office of Science helps guarantee that energy technology development is being conducted with the benefit of advanced scientific knowledge and that the basic research programs are focused in areas directly relevant to energy systems.

Impacts—Select Examples

Against this backdrop, DOE's basic science programs have contributed substantially to the energy R&D mission of the Department. For example, in the past 50 years, 71 SC-supported researchers have received Nobel Prizes—a total that far surpasses that of any other public or private institution.

A long term study of R&D 100 Awards, considered the premier indicator of new technologies supported by private and public sector institutions, showed that SC-funded technologies dominate Award winners. During the period from 1963-1996, DOE received 62 percent of all R&D 100 Awards given to the Federal government. SC-funded research has received 177 awards (41 percent of the DOE total/25 percent of the Federal total), making the Office of Science the most frequent recipient in the Federal government. Comparisons with recipients in private industry and academia show similar results.

Below are some select examples that illustrate the energy impacts of SC-funded research in basic science:

- Development of the current generation of high energy and power lithium and lithium ion batteries from research into non-aqueous electrolytes.
- Batteries half the thickness of saran wrap stemming from research into ion transport in glassy solids.
- Improved natural gas separation processes stemming from research into reverse selectivity inorganic membranes.
- Enhanced separation of heavy elements in the nuclear industry from research on actinide separations and related research.
- Ability to produce new, valuable polymers from research into new metallocene catalysts.
- Original discovery of a new class of carbon materials—buckeyballs.
- Potentially new ways to store hydrogen through the discovery of new graphite nanofibers that can store three times their weight of hydrogen.
- Major improvements in the toughness of silicon carbide ceramics.
- Breakthrough processing of aerogel films, ideal insulating materials.
- Design of more reliable joints between ceramics and metals from improved finite element models.
- Research leading to the commercialization of gelcasting for molding near-net shape ceramic parts.
- New and better future diesel engine designs stemming from computational and technology research into models that predict soot generation.

- Discovery of a new marker for efficient combustion.
- Testing and development of nontoxic corrosion inhibitors using a special "vibration pole."
- Breakthrough levels in energy production from fusion plasma experiments.
- New genetic manipulation techniques to improve the properties of bacteria that are capable of producing methane.
- Lignin depolymerizing enzymes with the potential for an effective "green" technology in pulp and paper production.
- Development of a new catalytic control system for a lean burn engine.
- Development of a photovoltaic cell that holds three world records for efficiency, stemming from collaborative research between EE and SC.
- Improved miniaturization through research into nanowires, "magic structures," and conductance quantization.
- A tenfold increase in the electrical conductivity of semiconductors through research into gallium injection.
- Improved imaging of pore spaces in sandstone for oil recovery through research into synchrotron x-ray micro tomography.
- Artificial photosynthesis through research into light-matter interactions and proton motive force.
- Improved high temperature superconductors through research into pairing mechanisms and vortex physics.