

U.S. Department of Energy-

A TRADITION OF EXCELLENCE IN SCIENCE AND TECHNOLOGY



The Office of Basic Energy Sciences (BES) is the Nation's foremost sponsor of fundamental research in broad areas of materials sciences, chemical sciences, geosciences, biosciences, and engineering sciences. The

BES program underpins Department of Energy (DOE) missions in energy and the environment, advances energy-related basic science on a broad front, and provides unique national research facilities for the scientific community. BES-sponsored researchers and students receive extensive recognition and have shared in four Nobel prizes within the last decade:

- Yuan Tseh Lee, UC Berkeley, for "dynamics of chemical elementary processes" (Chemistry, 1986)
- Donald J. Cram, UC Los Angeles, for "development of molecules with structurally specific interaction of high specificity" (Chemistry, 1987)
- Clifford G. Shull, MIT, for "pioneering contributions to the development of neutron scattering techniques for studies of condensed matter" (Physics, 1994)
- Frank Sherwood Rowland, UC Irvine, for "work in atmospheric chemistry, particularly concerning the formation and decomposition of ozone" (Chemistry, 1995)

BES research undergoes rigorous peer evaluation through competitive grant applications, program reviews involving outside experts, and advisory panels composed of leading scientists. BES has successfully completed more than \$1B in world-class scientific facility construction over the past decade on schedule and within budget. Program direction costs are less than 1.5% of the research budget.



Neutron scattering was pioneered at Oak Ridge National Laboratory in the 1950s by Nobel Laureate C. G. Shull (standing) and E. O. Wollan.



Nobel Laureate Y. T. Lee's crossed molecular beam experiments revolutionized the fundamental understanding of chemical reactions.



BES supports energy-related basic research at universities, national laboratories, and major national facilities.

Cover: Combustion research addresses critical issues in energy utilization and the environment.

A UNIQUE ROLE IN THE NATION'S RESEARCH EFFORT

BES is uniquely responsible for basic research in the natural sciences leading to new and improved energy technologies. BES supports fundamental research in areas related to energy resources, production, conversion, and efficiency and to the mitigation of the adverse impacts of energy production and use. Through its diversified portfolio and system of laboratory and university programs, BES promotes interdisciplinary research and the integration of basic and applied science. Encompassing more than 2400 researchers in 200 institutions nationwide, the program includes extensive interactions at the interagency, national, and international levels, as well as over 800 collaborations with industry.

BES is responsible for the planning, construction, and operation of many of the Nation's most sophisticated research facilities, including third-generation synchrotron light sources and high-flux neutron sources as well as specialized facilities for microcharacterization, materials synthesis, combustion research, and ion beam studies. These facilities are unmatched in the world in breadth of capabilities and numbers of scientific users. BES facilities have an enormous impact on science and technology, ranging from determinations of the structure of superconductors and biological molecules to the development of wear-resistant prostheses, from atomic-scale characterization of environmental samples to elucidation of geological processes, and from the production of unique isotopes for defense applications and cancer therapy to the development of new medical imaging technologies.



The Advanced Photon Source at Argonne National Laboratory is the nation's most intense synchrotron x-ray source.



BES research facilities serve over 4500 researchers from universities, industry, and government laboratories each year.

ADVANCING THE SCIENTIFIC FRONTIER

Advanced Alloys and Ceramics. Materials are critical for the technological future of the Nation. Basic research is essential for controlling materials performance and creating new materials. BES excels in synthesis and processing research, micro-characterization, and the multidisciplinary R&D required for the development of high-performance alloys, ceramics, and novel materials for a wide variety of energy-related applications.

Polymers. Widely used in transportation technologies, corrosive environments, and microelectronics, polymers are macromolecules made up of sequences of thousands of atoms. BES combines synthesis and processing; research with theory and microcharacterization to develop novel polymeric molecules and processing methods and to elucidate structure-property relationships.

Geosciences. The identification and recovery of energy resources and the geological disposal of radioactive and toxic wastes have enormous economic and social impacts. BES emphasizes theoretical, experimental, and field-based investigations on rock-fluid mechanics and subsurface migration. This research lies at the heart of a wide range of issues including subsurface contaminant transport, nuclear waste isolation, petroleum production, and geothermal resource development.

Energy Biosciences. Plants and photosynthetic microorganisms are solar energy transducers that produce fuels and useful chemicals. BES supports fundamental research into the mechanisms of how plants and microorganisms grow, metabolize, and reproduce. This research provides the foundation for the use of biological systems in energy-related technologies ranging from the production of biodegradable plastics to the conversion of biomass to potential fuels.

Heavy Element Chemistry. Heavy element chemistry provides fundamental understanding on the behavior of elements heavier than uranium in the environment. This research merges chemistry and physics, advanced spectroscopic techniques, and unique BES facilities to address related scientific issues in plutonium processing, nuclear waste isolation, nuclear weapons safety, remediation of contaminated sites, and the transport of plutonium in the environment.



Clockwise from upper left: high-performance intermetallic alloys, positron annihilation studies of surfaces, laser spectroscopy for trace element analysis, plasma processing, omnidirectional robotics platform, energy bioscience plant research, subsurface migration of fluids.

IN SUPPORT OF THE ENERGY MISSION



Surface Physics. BES supports multidisciplinary research in surface physics and chemistry that contributes to the development of solid and molecular catalytic materials, the understanding of structure-property relationships at surfaces, the development of ion beam and other surface processing techniques for novel semiconductors and thin films and for enhanced corrosion and wear performance, and the development of new techniques for probing surfaces at the atomic level.

Molecular Environmental Science. Fundamental research on the molecular-scale processes that affect environmental contaminants is key to understanding their fate and transport in the environment, their uptake in the biosphere, and their remediation and management. BES is the leader in the development of this new interdisciplinary field which provides a science base for the management of contaminants in soils, natural waters, and the atmosphere.

Advanced Separation Science. Chemical separations are vital to energy savings and process improvements in energy and environmental technologies. BES draws from chemistry, engineering, and computational science to advance separations science from the identification of new chemical structures for membranes to detailed molecular dynamics simulations of selective permeation processes.

Combustion Research. Fundamental combustion research is critical to improving the efficiency of combustion processes while reducing their environmental impact. BES combines theoretical and experimental research on molecular energetics, chemical process dynamics, and reaction rates to develop quantitative models of combustion-generated pollutants and flames.

Solar Energy Conversion. Photochemical and photophysical energy research develops new approaches to utilize light in energy processes. BES forges links between theory and experiment to develop photoactive molecules and materials, to uncover the mechanism of photosynthesis, and to develop more efficient photovoltaic materials.

Engineering Sciences. Innovative engineering approaches are needed to meet many challenges in energy and environmental technology. BES engineering research extends underlying knowledge in energy-related areas including fluid and solid mechanics, heat transfer, intelligent machines, instrumentation and diagnostics for process and environmental control, and dynamical systems for engineering applications.

SCIENCE SERVING THE PRESENT



Basic Energy Sciences research touches people's lives in countless ways-from advances in energy and environmental technologies, to new materials and processes, to important spin-offs in industry and medicine. The few examples provided here

illustrate the breadth and impact of BES discoveries.

Magnetic Materials. BES researchers have shown that making improvements in the processing of the core magnets used in transformers reduces energy losses by up to a factor of 10. Their results suggest that postprocessing improvements (e.g., surface annealing and laser scribing) could enhance the magnetic properties of transformer materials, significantly reducing the estimated \$1B lost each year as a result of inefficiency in these materials.

Superconductors. BES researchers have developed the first practical application of the new hightemperature superconductors. The device, called a superconducting quantum interference device or SQUID, is a magnetometer capable of measuring minute magnetic fields, such as those emanating from the human heart and brain. The SQUID can also be used for nondestructive evaluation of materials for hidden flaws.

Catalysts. Enzymes valued at billions of dollars per year are used as catalysts, in industrial processes, in pharmaceuticals, and as specialty chemicals. BES researchers have developed a novel carbohydrate-based polymer that stabilizes a wide variety of proteins, including enzymes and antibodies, by wrapping around the protein surface to provide a unique and stabilizing microenvironment. The coatings allow enzymes to remain active in hostile industrial environments and prolong their useful lifetimes.

Wear-Resistant Surfaces. BES research on corrosion and wear has led to the development of an ion implantation technique that is used each year in processing more than 100,000 artificial hips, knees, and other orthopedic devices. This surface treatment produces remarkable improvement in the wear resistance of such devices, extending their useful lifetimes and increasing reliability.



Clockwise from upper left: superconducting SQUID, zeolite molecular structure, whisker-toughened ceramic, chemical vapor deposition model, synchrotron x-ray angiography, stabilized enzyme catalysts, ion-implanted hip joint.

AND SHAPING THE FUTURE



Molecular Structure. The Nation's largest petroleum and chemical companies use BES synchrotron facilities and neutron sources to gather information about the three-dimensional structure of molecules involved in their manufacturing processes. Knowledge about the local environment of specific atoms in zeolite catalysts, **for** example, could lead to more efficient petroleum refining.

Solar Cells. A solar cell developed by BES researchers has set a world record for efficiency-29.5%. This achievement, if duplicated in production cells, will significantly broaden the applications for solar electric power.

Toughened Ceramics. BES research has contributed to the development of new tough ceramics that are finding a wide range of industrial applications including high-speed cutting tools, ceramic die inserts, and hot gas filters. According to independent market assessments, sales of these products are expected to exceed \$200M annually by 2000. Fundamental ceramic research, including modeling, interface characterization, and process science, has been essential in determining how to control the microstructures and the properties in these ceramics.

Process Modeling. BES experimental research is extended through sophisticated numerical simulations which can mimic the behavior of materials in automobile crashes or the transport of contaminants in aquifers. A model developed to study the fundamental chemical interactions that occur during chemical vapor deposition, an important technological processing technique used in fabrication of semiconductors and other types of thin films, is widely used in industry. The model helps researchers and process managers to understand vapor phase chemistry.

Imaging Science. Synchrotron light sources produce X rays able to probe, analyze, and image materials on a near nanoscopic scale-including semiconductors, magnetic materials, ceramics, polymers, and biological molecules. The unique properties of these X rays result in a wide range of applications from medical research aimed at eliminating the dangerous catheterization required by x-ray angiography for diagnosing and monitoring heart disease to looking at individual bits a computer disk while developing magnetic media with more storage capacity.

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BES supports research at 200 institutions nationwide.



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