Basic Energy Sciences

Funding Profile by Subprogram

	(dollars in thousands)	
	FY 2010 Current Appropriation	FY 2012 Request
Basic Energy Sciences		
Materials Sciences and Engineering	353,423	459,952
Chemical Sciences, Geosciences, and Biosciences	287,480	394,717
Scientific User Facilities	803,825	978,931
Subtotal, Basic Energy Sciences	1,444,728	1,833,600
Construction	154,240	151,400
Total, Basic Energy Sciences	1,598,968[a]	1,985,000

Public Law Authorizations:
Public Law 95–91, "Department of Energy Organization Act", 1977
Public Law 108–153, "21st Century Nanotechnology Research and Development Act 2003"
Public Law 109–58, "Energy Policy Act of 2005"
Public Law 110–69, "America COMPETES Act of 2007"
Public Law 111–358, "America COMPETES Act of 2010"

Program Overview

Mission

The mission of the BES program is to support fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels in order to provide the foundations for new energy technologies and to support DOE missions in energy, environment, and national security.

Background

Our ability to discover and transform the material resources that nature provides has shaped history and built civilizations. From prehistoric hunters and gatherers, who utilized wood-burning fires and fashioned tools from stone, to modern nations that run on processes powered primarily by coal and oil, progress has been marked by advanced technologies designed to make better use of Earth's resources. Today, science and technology are increasingly at the heart of many critical societal, political, and economic issues that surround the energy security and sustainability of our nation.

The energy challenges of the next century will fundamentally depend on scientific discovery and technological innovation. The lessons of the previous century illustrate that major breakthroughs in energy technologies are largely built on a deep foundation of basic research advances. Solar photovoltaic technology has its roots in Einstein's early twentieth-century paper on the photoelectric effect. The development of nuclear energy would have been impossible without the atomic science pioneered by Einstein and others. Even the electronics used to render today's internal combustion engine more efficient have their root in the transistor, whose development was critically dependent on concept of quantum mechanics. At the core of these advances is the ability to create new materials using

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[a] Total is reduced by $37,532,000, $33,511,000 of which was transferred to the Small Business Innovation Research (SBIR) program, and $4,021,000 of which was transferred to the Small Business Technology Transfer (STTR) program.

sophisticated synthetic and processing techniques, precisely define the atomic arrangements in matter, and control physical and chemical transformations.

The research disciplines that the BES program supports—condensed matter and materials physics, chemistry, geosciences, and aspects of physical biosciences—are those that discover new materials and design new chemical processes. These disciplines touch virtually every aspect of energy resources, production, conversion, transmission, storage, efficiency, and waste mitigation. BES research provides a knowledge base to help understand, predict, and ultimately control the natural world and serves as an agent of change in achieving the vision of a secure and sustainable energy future.

The BES program is one of the nation's largest sponsors of research in the natural sciences. In FY 2010, the program funded research in more than 170 academic institutions located in 50 states and in 14 DOE laboratories located in 12 states. Thus, approximately 40% of the BES program's research activities are sited at academic institutions. The BES program also supports world-class open-access scientific user facilities that provide outstanding capabilities for imaging; for characterizing materials of all kinds from metals, alloys, and ceramics to fragile biological samples; and for studying the chemical transformation of materials. These facilities are used to correlate the microscopic structure of materials with their macroscopic properties, which provides critical insights to their electronic, atomic, and molecular configurations, often at ultrasmall length and ultrafast time scales.

The energy systems of the future—whether they tap sunlight, store electricity, or make fuel from splitting water or reducing carbon dioxide—will revolve around materials and chemical changes that convert energy from one form to another. Such materials will need to be more functional than today's energy materials. To control chemical reactions or to convert a solar photon to an electron requires coordination of multiple steps, each carried out by customized materials with designed nanoscale structures. Such advanced materials are not found in nature; they must be designed and fabricated to exacting standards using principles revealed by basic science.

The 20th century witnessed revolutionary advances in the physical sciences, bringing remarkable discoveries such as high-temperature superconductors, electron microscopy with atomic resolution, and carbon nanotubes that combine the strength of steel with the mass of a feather. Observational science is now giving birth to the science of control, where accumulated knowledge derived from observations is used to design, initiate, and direct the chemical and physical behavior of materials at atomic and nanoscale. BES-supported research stands at the dawn of an age in which materials can be built with atom-by-atom precision and computational models can predict the behavior of materials before they exist. These capabilities, unthinkable only a few decades ago, create unprecedented opportunities to revolutionize the future of sustainable energy applications and beyond, from information management to national security.

Subprograms

To accomplish its mission and address the scientific challenges outlined above, the BES program is organized into three subprograms: Materials Sciences and Engineering; Chemical Sciences, Geosciences, and Biosciences; and Scientific User Facilities.

The *Materials Sciences and Engineering* subprogram supports research that explores the origin of macroscopic material behaviors and their fundamental connections to atomic, molecular, and electronic structures. At the core of the subprogram is the quest for a paradigm shift for the deterministic design and discovery of new materials with novel structures, functions, and properties. To accomplish this goal, the portfolio stresses the need to probe, understand, and control the interactions of phonons, photons, electrons, and ions with matter to direct and control energy flow in materials systems over multiple time and length scales. Such understanding and control are critical to science-guided design of highly efficient energy conversion processes, such as new electromagnetic pathways for enhanced light emission in solid-state lighting and multi-functional nanoporous structures for optimum charge transport in batteries and fuel cells. This subprogram also seeks to conceptualize, calculate, and predict processes underlying physical transformations, tackling challenging real-world systems—for example, materials with many atomic constituents, with complex architectures, or that contain defects; systems that exhibit correlated emergent behavior; and systems that are far from equilibrium. Such understanding will be critical to developing predictive capability for complex systems behavior, such as in superconductivity and magnetism. The subprogram also supports the development and advancement of the experimental and computational tools and techniques that in turn enable the understanding of the behaviors of materials, especially their reactivity under the full range of extreme conditions and the ability to predict the structure and properties of formed phases. Finally, the subprogram exploits the interfaces between physical and biological sciences to explore bio-mimetic processes as new approaches to novel materials design.

The *Chemical Sciences, Geosciences, and Biosciences* subprogram supports research that explores fundamental aspects of chemical reactivity and energy transduction over an enormous range of scale and complexity. Phenomena are studied over spatial scales from the sub-nanometer, as defined by the structure of atoms and molecules, to kilometers, appropriate to the behavior of subsurface geological structures, and over time scales defined by the motions of electrons in atoms, attoseconds (10^{-18} seconds), to millennia over which geological change must be understood. At the heart of this research lies the quest to understand and control chemical reactions and the transformation of energy at the molecular scale in systems ranging from simple atoms and molecules, to active catalysts, to complex biochemical or geochemical substances. At the most fundamental level, the development and understanding of the quantum mechanical behavior of electrons, atoms, and molecules in the 20th century has now evolved into the ability to control and direct such behavior to achieve desired results, such as the optimal conversion of solar energy into electronic excitation in molecular chromophores or into the creation of multiple charge carriers in nanoscale semiconductors. This subprogram also seeks to extend this new era of control science to include the capability to tailor chemical transformations with atomic and molecular precision. Here, the goal is to achieve fully predictive assembly and manipulation of larger, more complex chemical systems, such as interfacial catalysis, at the same level of detail now known for simple molecular systems. Finally, this subprogram seeks ultimately to achieve a molecular level understanding and control of the emergent and highly non-equilibrium behavior of biological and geological systems through the application of state-of-the-art experimental and computational tools.

The *Scientific User Facilities* subprogram supports the operation of a geographically diverse suite of major facilities that provide researchers unique tools to advance a wide range of sciences. These user facilities are operated on an open access, competitive merit review, basis, enabling scientists from every state and of many disciplines from academia, national laboratories, and industry to utilize the facilities' unique capabilities and sophisticated instrumentation. These large-scale user facilities consist of a complementary set of intense x-ray sources, neutron scattering centers, electron beam characterization capabilities, and research centers for nanoscale science. These facilities probe materials in space, time, and energy with the appropriate resolutions that can interrogate the inner workings of matter—transport, reactivity, fields, excitations, and motion—to answer some of the most challenging grand science questions. Taking advantage of the intrinsic charge, mass, and magnetic characteristics of x-rays, neutrons, and electrons, these tools offer unique capabilities to help understand the fundamental aspects of the natural world. The subprogram recognizes that at the heart of scientific discovery lies advanced tools and instruments. The continual development and upgrade of the instrumental capabilities includes new x-ray and neutron experimental stations, improved core facilities, and new stand-alone instruments. The subprogram also manages a research portfolio in accelerator and detector development to explore technology options for developing the next generations of x-ray and neutron sources. Collectively, these user facilities and enabling tools produce a host of important research results that span the continuum from basic to applied research and embrace the full range of scientific and technological endeavors, including chemistry, physics, geology, materials science, environmental science, biology, and biomedical science. These capabilities offer critical scientific insights for the discovery and design of advanced materials and novel chemical processes with broad societal impacts, from energy applications to information and biomedical technologies.

Benefits

The BES program supports basic research that underpins a broad range of energy technologies. Research in materials sciences and engineering leads to the development of materials that improve the efficiency, economy, environmental acceptability, and safety of energy generation, conversion, transmission, storage, and use. For example, advances in superconductivity have been introduced commercially in a number of demonstration projects around the country. Improvements in alloy design for high temperature applications are used in commercial furnaces and in green technologies such as lead-free solder. Research in chemistry has led to advances such as efficient combustion systems with reduced emissions of pollutants; new solar photoconversion processes; improved catalysts for the production of fuels and chemicals; and better separations and analytical methods for applications in energy processes, environmental remediation, and waste management. Research in geosciences results in advanced monitoring and measurement techniques for reservoir definition and an understanding of the fluid dynamics of complex fluids through porous and fractured subsurface rock. Research in the molecular and biochemical nature of photosynthesis aids the development of solar photo-energy conversion.

The BES program also plays a major role in enabling the nanoscale revolution. The importance of nanoscience to future energy technologies is clearly reflected by the fact that all of the elementary steps of energy conversion (e.g., charge transfer, molecular rearrangement, and chemical reactions) take place on the nanoscale. The development of new nanoscale materials, as well as the methods to characterize, manipulate, and assemble them, create an entirely new paradigm for developing new and revolutionary energy technologies.

Program Planning and Management

Inputs to program planning and prioritization include overall scientific opportunity, projected investment opportunity, DOE mission need, and Administration and Departmental priorities. Many long-range planning exercises for elements of the BES program are performed under the auspices of the Basic Energy Sciences Advisory Committee (BESAC). During the past few years, BESAC has provided advice on new directions in nanoscale science and complex systems; on the operation of the major scientific user facilities; on the need for new, next-generation facilities for x-ray, neutron, and electron-beam scattering; on performance measurement; on the quality of the BES program management and its consequent impacts on the program portfolio; on new directions in research relating to specific aspects of fundamental science such as catalysis, biomolecular materials, and computational modeling at the nanoscale; on the fundamental research challenges posed by the Department's energy missions; on a 20-year roadmap for BES facilities; and on theory and computation needs across the entire portfolio of BES research.

Of particular note is the 2003 BESAC report, *Basic Research Needs to Assure a Secure Energy Future*, which was the foundation for ten follow-on Basic Research Needs workshops supported by BES in the areas of 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 applications. Together these workshops attracted over 1,500 participants from universities, industry, and DOE laboratories. BESAC was charged with summarizing the results of these ten workshops and relating this summary to the science themes identified in the 2007 BESAC Grand Challenges study. A report, entitled *New Science for a Secure and Sustainable Energy Future*, was released in December 2008. The report highlighted the magnitude of the challenges in the realm of energy and environment facing the U.S and the importance of fundamental science to finding transformational solutions.

As a follow up to the series of Basic Research Needs workshops, BESAC was charged to assess basic research opportunities that will have more immediate impact on energy applications, and specifically to address strengthening the linkages between the basic research and industry communities. The basic science needs of industry are often more narrowly focused on solving specific nearer-term roadblocks to progress in existing and emerging clean energy technologies. To better define these issues and identify specific barriers to progress, a wide cross-section of scientists and engineers from industry, universities, and national laboratories participated in a workshop to delineate the basic science Priority Research Directions most urgently needed to address the roadblocks and accelerate the innovation of clean energy technologies. A key conclusion of the report, entitled *Science for Energy Technology: Strengthening the Link between Basic Research and Industry*, is that in addition to the decadal challenges defined in the Basic Research Needs reports, specific research directions addressing industry roadblocks are ripe for further emphasis. Another key conclusion is that identifying and focusing on specific scientific challenges and translating the results to industry requires more direct feedback and communication and collaboration between industrial and BES-supported scientists. The report also recognized that the suite of BES scientific user facilities play a key role in advancing the science of clean energy technology.

Together these reports describe a continuum of research spanning the most fundamental questions of how nature works to the questions that address technological show-stoppers in the applied research programs supported by the DOE technology offices as well as by industry. Dealing with these issues requires breakthrough advances with new understanding, new materials, and new phenomena that will come from fundamental science. These reports will continue to inform the BES research agenda to bring frontier research to bear on addressing the Department’s mission in science and energy.

Planning for the facilities of the BES program is also an ongoing activity. The BES program has a long tradition of planning, constructing, and operating facilities well. During the past ten years, the BES program has delivered nearly $2 billion of facilities and upgrades on schedule and within budget. Among others, this includes the Spallation Neutron Source, the complete reconstruction of the Stanford Synchrotron Radiation Lightsource, five Nanoscale Science Research Centers, the Linac Coherent Light Source, and numerous instrument fabrication projects. BESAC sponsored a workshop *Next-Generation Photon Sources for Grand Challenges in Science and Energy* to explore the scientific frontiers that could be tackled with next generation photon sources. The workshop identified new research opportunities in materials, chemistry, biology, medicine, environment, and physics for science and energy that can be addressed with diffraction, excitation, and imaging by photons. BES built on this foundation and conducted two follow-on workshops to assess the technical readiness of various approaches for 4th generation light sources, including compact light sources, and the corresponding R&D needs in 2009 and 2010. It is expected that the output of these workshops will help set the course for photon science facilities for the next decade.

All research projects supported by BES undergo regular peer review and merit evaluation based on procedures set down in the Code of Federal Regulations, 10 CFR Part 605, for the extramural grant program and in an analogous process for the laboratory programs and scientific user facilities. The BES peer review process evaluates the following four criteria, in order of decreasing importance: scientific and/or technical merit of the project, appropriateness of the proposed method or approach, competency of the personnel and adequacy of proposed resources, and reasonableness and appropriateness of the proposed budget. The criteria for review may also include other appropriate factors established and announced by BES.

Facilities are reviewed using external, independent review committees operating according to the procedures established for peer review of BES laboratory programs and facilities. Important aspects of the reviews include assessments of the quality of research performed at the facility, the reliability and availability of the facility, user access policies and procedures, user satisfaction, facility staffing levels, R&D activities to advance the facility, management of the facility, and long-range goals of the facility. The outcomes of these reviews helped improve operations and develop new models of operation for all BES scientific user facilities.

Facilities that are in design or construction are reviewed according to procedures set down in DOE Order 413.3B "Program and Project Management for Capital Assets" and in the Office of Science "Independent Review Handbook." In general, once a project has entered the construction phase, it is reviewed with external, independent committees approximately biannually. These Office of Science construction project reviews enlist experts in the technical scope of the facility under construction and its costing, scheduling, and construction management.

BESAC also reviews the major elements of the BES program annually using Committees of Visitors (COVs). The first COV review of BES was conducted in 2002, and all elements of the BES program have been reviewed once every three years on a rotating schedule. COVs assess the efficacy and quality of the processes used to solicit, review, recommend, monitor, and document proposal actions; and the quality of the resulting portfolio, specifically the breadth and depth of portfolio elements and the national and international standing of the elements. The latest COV was held on April 6–8, 2010, on the Scientific User Facilities subprogram, and the next COV will be in April 2011 on the Chemical Sciences, Geosciences, and Biosciences subprogram. All BES COV reports are available on the BES web site.

Information and reports for all of the above mentioned advisory and consultative activities are available on the BES website. Other studies are commissioned as needed using the National Academies' National Research Council and other independent groups.

Basic and Applied R&D Coordination

As is demonstrated by the depth and scope of the Basic Research Needs workshop series, the BES program is committed to R&D integration. These workshops and the follow-on solicitations seek to partner the BES program with its counterparts in the DOE technology offices and NNSA.

Many activities facilitate cooperation and coordination between BES and the applied research programs, including joint efforts in strategic planning, solicitation development, peer reviews, and program contractors meetings. For example, in hydrogen research, BES has actively engaged with the Offices of Energy Efficiency and Renewable Energy, Fossil Energy, and Nuclear Energy to coordinate activities such as budget submissions, solicitation topic selections and proposal reviews, posture plan development, and joint contractors meetings. BES participates in the DOE Hub Working Group, which meets regularly with representatives from the Office of Energy Efficiency and Renewable Energy and the Office of Nuclear Energy to provide integrated programmatic oversight and promote commonality across the three DOE Energy Innovation Hubs that were initiated in FY 2010—Fuels from Sunlight, Modeling and Simulation for Nuclear Reactors, and Energy Efficient Building Systems Design. BES also participates in interagency coordination activities, such as the Interagency Working Group on Hydrogen and Fuel Cells led by the White House Office of Science and Technology Policy; the Hydrogen Technical Advisory Committee (HTAC), a Federal Advisory Committee established by the Energy Policy Act of 2005 to advise the Secretary of Energy on issues related to hydrogen and fuel cell research, development, demonstration, and deployment; and the Hydrogen and Fuel Cell Interagency Task Force consisting of senior agency representatives across the Federal Government. BES also coordinates with the Office of Energy Efficiency and Renewable Energy and the Office of Electricity Delivery and Energy Reliability on electrical energy storage research for transportation and grid-level storage, respectively. BES has involved program managers in both offices in regular information exchange meetings and in developing a preliminary coordination plan in electrical energy storage. BES coordinates with DOE technology offices on the Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) program, including the topical area planning, solicitations, reviews, and award selections. Since FY 2007, BES has worked with the Office of Electricity Delivery and Energy Reliability to initiate SBIR awards in electrical energy storage for grid applications.

At the program manager level, there have been regular intra-departmental meetings for information exchange and coordination on solicitations, program reviews and project selections in research areas such as biofuels derived from biomass; solar energy utilization; hydrogen production, storage, and use; building technologies, including solid-state lighting; advanced nuclear energy systems and advanced fuel cycle technologies; vehicle technologies; improving efficiencies in industrial processes; and superconductivity for grid applications. These activities facilitate cooperation and coordination between BES and the technology offices and defense programs. DOE program managers have also established formal technical coordinating committees that meet on a regular basis to discuss R&D programs with wide applications for basic and applied programs. Additionally, technology offices staff participate in reviews of BES research, and BES staff participate in reviews of research funded by the technology offices and ARPA-E.

The Department’s national laboratory system plays an important role in the ability of BES to effectively integrate research and development by providing opportunities to collocate activities at the laboratories. Co-funding and co-siting of research by BES and DOE technology programs at the same institutions, such as the DOE laboratories or universities, has proven to be a valuable approach to facilitate close integration of basic and applied research. In these cases, teams of researchers benefit by sharing of resources, expertise, and knowledge of research breakthroughs and program needs.

Budget Overview

In FY 2012, the BES program will support expanded efforts in basic research related to transformational clean energy technologies. These new directions derive from the series of “Basic Research Needs” workshop reports and the follow-on workshop reports by the Basic Energy Sciences Advisory Committee. As recognized in the series of workshop reports, clean energy technologies are in their infancy compared to traditional fossil fuel-based technologies, and they have many scientific and technological challenges to overcome in order to operate at their full potential. The reports have defined the decadal science challenges whose solutions will create comprehensive understanding and control of clean energy phenomena; they have also been instrumental in guiding the establishment of the 46 Energy Frontier Research Centers (EFRCs), which exemplify the pursuits of the broad-based science challenges for energy applications. Complementary to such broad-based research efforts are opportunities to focus more specifically on limitations of performance in existing clean energy technologies. The limitations can be overcome through targeted basic research efforts aimed at understanding the phenomena underlying performance limitations and contributing innovations based on scientific understanding that remove barriers to technological progress. The requested increases in FY 2012 for clean energy are primarily guided by the recent BESAC report *Science for Energy Technology: Strengthening the Link between Basic Research and Industry*, which stresses the importance of sustained efforts of testing new concepts, identifying roadblocks, and pursuing scientific and technical solutions to accelerate transformative advances for targeted impact on cost, reliability, and performance—in a way similar to the development of information technology, in which generations of innovative advances in silicon-based devices yielded Moore's Law and game-changing breakthroughs.

In order to achieve the President's challenge of generating 80% of America's electricity from clean energy sources by 2035, the FY 2012 budget request includes funding for integrated R&D activities across the Department's technology programs and the Office of Science. The DOE technology programs will manage applied research, development, and deployment efforts to gain and apply knowledge to achieve identified near-to-mid-term goals. The basic research work within BES is selected in clean energy areas where an understanding of the fundamental phenomena is necessary to achieve game-changing discoveries for mid-to-longer-term technological innovation.

Our science based approach for creating transformational improvements in clean energy technologies consists of increasing basic research on a set of interrelated energy issues: non-carbon sources, carbon capture and sequestration, transportation and fuel switching, transmission and energy storage, and efficiency. These basic research efforts will be conducted in coordination with the complementary R&D activities in the following DOE programs: Office of Energy Efficiency and Renewable Energy, Office of Nuclear Energy, Office of Electricity Delivery and Energy Reliability, Office of Fossil Energy, and the National Nuclear Security Administration. The FY 2012 budget contains increases to BES research in the following areas, as detailed in this budget submission and summarized below.

- ***Non-carbon Sources:***
  - *Solar Electricity from Photovoltaics – Fundamental Science of Interfaces and Degradation* (+$8,000,000). Many critical issues that surround the performance, cost, and reliability of solar photovoltaics (PV) are associated with interfaces: p-n junctions, device contacts, light and carrier reflectors, tunnel junctions, passivation and buffer layers, grain boundaries in polycrystalline semiconductors, and packaging materials. Technology development in PV interfaces has been largely empirical in nature. Greatly improved characterization tools provide a unique opportunity to probe PV interfaces in situ and enable new research opportunities for improved fundamental understanding of their behavior. Fundamental research is also required to improve the scientific basis for understanding the mechanisms by which PV modules are degraded. Particular emphasis will be place on degradation and the long-term effects of impurity diffusion processes.
  - *Advanced Nuclear Energy – Basic Actinide Chemistry Research for Fuel Cycles* (+$8,000,000). New research is proposed to significantly advance fundamental understanding of actinide molecules and their chemistry, with broad impacts for nuclear reactor fuels, waste forms, and separations techniques. Proposed research includes development of more sophisticated theoretical and experimental tools for the understanding of the structure and bonding of actinide species with an emphasis on separation chemistry addressing the multiplicity of chemical forms and oxidation states for actinides in fuels, solutions, and waste forms. New characterization and computational tools can play particularly important roles in addressing these challenges. These tools offer the opportunity to transform and accelerate the fundamental chemistry that underpins technology development for advanced nuclear energy systems.
  - *Materials under Extreme Environments* (+$15,000,000). The physical processes that occur in materials under extreme nuclear technology environments span time scales from femtoseconds to decades and proceed over length scales ranging from atomistic to meters. These processes must be understood for real, engineered materials including complex alloys, materials with defects and impurities, materials with complex microstructures, and ranging from actinides to metals to

composites. Research in this area will focus on understanding, modeling, and designing radiation-resistant materials that maintain all of the required physical properties after prolonged exposure. Materials discovery will include nanoscale design of new materials, including self-healing potential to limit the impact of defects generated in the extreme exposures in reactors. In situ experiments will be closely integrated with theoretical/computational efforts to develop a fundamental understanding of degradation mechanisms and kinetics over multiple length and time scales.

- ***Carbon Capture and Sequestration***
  - *Carbon Capture – Novel Molecular Design* (+$8,000,000). The objective of research in predictive modeling of carbon capture will be to gain significant advances in quantum chemical structure determination, intermolecular potentials, and molecular dynamics algorithms on CO_2 interactions with complex materials and minerals for efficient and cost-effect carbon capture and sequestration. Specific emphasis will be placed on the discovery and design of new materials that incorporate complex structures and functionalities tuned for optimum separation properties; understanding and controlling the atomic and molecular level interactions of the targeted species with the separation media; and tailored capture/release processes with alternative driving forces, taking advantage of a new generation of nanoscale materials.
  - *Carbon Sequestration – Multiscale Dynamics of Flow and Plume Migration* (+$8,000,000). Permanent storage of captured CO_2 through injection into deep underground geologic formations has been proposed as the most practical approach to store captured industrial scale carbon emissions. Significant scientific and technical challenges must be overcome to scale up sequestration methodologies reliably and safely to effective operational levels. A critical current limitation is the inaccuracy of models that seek to describe the migration of CO_2 in the subsurface, which require characterization over vast spatial scales under multiple geological sites. New research to improve field-scale models will emphasize the improved understanding of geologic processes and rates relevant to subsurface sequestration sites, including better understanding of reservoir-scale geochemistry; reactive flow and transport processes and rates; higher resolution geophysical measurement techniques; and more accurate simulation approaches for linking geochemical processes and geophysical responses across multiple spatial scales.
- ***Transportation and Fuel Switching***
  - *Energy Systems Simulation – Internal Combustion Engines (ESS-ICE).* (+$15,000,000). Research activities in this area will focus on predictive modeling of combustion in an evolving fuel environment, thus building on the science base for the development of simulation tools for advanced internal combustion engine design. Basic research in ESS-ICE will emphasize the development of two complementary, experimentally validated sets of codes: one for stochastic, in-cylinder engine processes and one that can reliably predict the temporal and spatial behavior of liquid fuel injection. These two areas have been identified as high priorities by the U.S. engine industry and lie on the critical path toward the complete transition from hardware-intensive, experience-based engine design to simulation-intensive, science-based design. This research will be particularly important for the economic design of high-efficiency, clean engines burning a variety of fuels, including biofuels.
  - *Batteries and Energy Storage Hub* (+$34,020,000). Initiated in FY 2010, the Energy Innovation Hubs are designed as a multidisciplinary effort that addresses critical science and technology

issues in an integrated manner. A Hub focuses teams of researchers in separate but collaborative research areas on overcoming scientific barriers to development of a complete energy system with potential for implementation into a transformative energy technology. In FY 2012, BES will support the continuation of the Fuels from Sunlight Hub and will initiate a new Hub on Batteries and Energy Storage. The Hub is aimed at developing electrochemical energy storage systems that safely approach theoretical energy and power densities with very high cycle life. These are systemic challenges, and the Hub will result in new materials, systems, and knowledge critical to developing a robust industrial base leading the next generation of energy storage technology, including that for transportation (e.g., batteries for plug-in hybrid and all electric vehicles). Knowledge gained in the Batteries and Energy Storage Hub could also contribute to grid-level or stationary energy storage, as noted in the *Transmission and Energy Storage* section below.

- ***Transmission and Energy Storage***
  - *Electric Power Grid – Enabling Materials Sciences* (+$4,000,000). The research activities will include development of advanced materials for normal and superconducting power transmission lines and electronic components and devices to control and link complex high voltage direct current networks. Additional research will be initiated for developing nano-materials and novel deposition processes to achieve improved properties for cost-effective, high-capability electric power distribution.
  - *Power Electronics* (+$3,500,000). The Nation's future electric systems will need cost-effective, reliable, high-capability power electronic components and devices to control and link complex high voltage networks, measure and control flow, and reduce energy losses in long-distance transmission. Power electronics are particularly important in interfacing new, renewable electrical power sources to the existing grid distribution systems. In particular, wide bandgap materials that permit single devices to control current flows at higher voltages with high efficiency could make power electronics affordable and enable efficient tools to control and manage electricity. Focus areas in basic materials research will be initiated in low defect density, wide bandgap semiconductors; magnetic materials for high frequency inductors, including non-rare earth based materials; and next generation dielectrics.
  - *Batteries and Energy Storage Hub* (same Hub as above). The Hub is aimed at developing electrochemical energy storage systems that safely approach theoretical energy and power densities with very high cycle life. These are systemic challenges, and the Hub will result in new materials, systems, and knowledge critical to developing a robust industrial base leading the next generation of energy storage technology, including that for grid and other stationary energy storage applications. Knowledge gained in this Hub could also contribute to electrical energy storage for vehicle applications as noted in the *Transportation and Fuel Switching* section above.
- ***Efficiency***
  - *Advanced Solid-state Lighting – Novel Light Emitting Diodes* (+$8,000,000). Solid-state lighting is the direct conversion of electricity to visible white light using inorganic semiconductor materials, organic materials or hybrid combinations. By avoiding the indirect processes characteristic of traditional incandescent and fluorescent lighting that generate heat, solid state lighting can greatly improve the conversion efficiency. There is no known fundamental physical barrier to achieving ultrahigh efficiencies for visible white light. The proposed research will focus on the design of new materials to control the flow of electrons, including research on understanding light-emitting organic and inorganic (and hybrid) materials and nanostructures,

control of the materials and nanostructure properties, research on interfacial issues between semiconductors, metals and organic materials and the development of a fundamental understanding of the processes that mediate the competing conversion of electrons to light and heat.

- *Energy Efficiency – Enabling Materials Sciences* (+$4,000,000). Buildings are responsible for nearly 40 percent of US primary energy use and 70 percent of electricity demand. Significant opportunities exist to improve building efficiencies. These include research on the development of novel building materials using nano-materials, novel deposition processes to achieve improved properties. Research on reducing electrical energy needs will include materials with optical and thermal properties that respond passively or controllably to external conditions for reducing heating and cooling demands, windows with controllable optical properties, and new lighting devices.

In addition to the aforementioned basic research opportunities in clean energy technologies, BES will initiate a new program in methane hydrates, which are naturally occurring combinations of methane and water that form at low temperatures and high pressures.

- *Methane Hydrates* (+$10,000,000). The emphasis of this activity will be on expanding the research base to characterize the formation mechanisms of gas hydrates and to understand and ultimately predict the environmental stability of hydrates at the systems level. This activity supports theory, multi-scale modeling and simulation, and experimental research in areas such as: the intermolecular forces that govern the structure and properties of methane hydrates; multi-phase behavior of hydrate-sediment systems; and studies of methane hydrates in the natural environment.

Increases in research funding also are requested as part of two inter-agency coordinated initiatives – *Computational Materials and Chemistry by Design* and *Nanoelectronics*. Both of these initiatives will provide the broad knowledge foundations critical for clean energy and other advanced technologies.

- *Computational Materials and Chemistry by Design* (+$40,000,000). As described in the Office of Science Workshop on *Computational Materials Science and Chemistry for Innovation*, over the past two decades, the United States has developed and deployed the world's most powerful collection of tools for the synthesis, processing, characterization, and simulation and modeling of materials and chemical systems at the nanoscale, from dimensions of a few atoms to a few hundred atoms across. We are at the threshold of a new era where control of these processes will transform our ability to understand and design new materials and chemistries. In turn, this predictive capability will transform technological innovation by accelerating the development and deployment of new materials and processes in products and manufacturing. Harnessing the potential of computational science and engineering for the discovery and development of materials and chemical processes is likely to have significant impact on our future industrial competitiveness.

  Computational Materials and Chemistry by Design is a multi-agency effort. DOE will lead in the development of new software tools and data standards that catalyze a fully integrated approach from material discovery to applications. New research efforts will be initiated to design materials with targeted properties and advanced chemical processes with high efficiencies through theory, computation, and modeling, as validated by precise experimental characterization. The era of modern technology requires understanding the complexity of materials and chemical assemblies well beyond that of the past centuries and beyond the current capabilities offered by experimental approaches alone. The need to accelerate the innovation cycle by taking advantage of the significant growth in modeling and high performance computing, underscores the critical importance of this request. Coupled with the goal of materials and chemistry by design is another critical goal for accelerating advances in energy technologies—the ability to accurately predict changes in materials and their properties associated with their use in a specific application, incorporating the effects of fabrication of materials into system components, influence of the environment in which materials are used, and extend the lifetime of their usage. Discovery of new materials and chemical assemblies with totally new properties and accurate lifetime predictions are crucial to generation, use, and advances in energy technologies, as well as to virtually all industries that use materials, both structural and functional, in their infrastructure and products—crossing the spectrum of transportation, electronics, buildings, chemicals and pharmaceuticals, health, and consumer products. This request envisions assembling integrated teams focused on key scientific knowledge gaps to develop new theoretical models, including their realization in reusable and broadly-disseminated software. Special attention will be paid to the development of powerful abstraction methods to enable the distillation of new physical laws bridging multiple length and temporal scales. The ultimate goal is to provide the Nation with a science-based computational tool set to rationally predict and design materials and chemical processes to gain a global competitive edge in scientific discovery and innovation.

- *Nanoelectronics* (+$10,000,000). *Nanoelectronics* is one of the signature activities of the National Nanotechnology Initiative coordinated by the National Science and Technology Council's subcommittee on Nanoscale Science, Engineering and Technology. BES research will focus on overcoming fundamental physics limitations of semiconductor processing and memory devices in two thrust areas: exploring new or alternative "state variables" for computing, e.g., other alternatives to charge transfer exploited by conventional transistors such as spintronics, and exploiting nanoscale processes and phenomena for quantum information science. These activities require the development of novel fabrication, processing, and instrumentation techniques, and new theoretical and modeling tools. This research will be informed by and coordinated with applied research in industries to identify the next generation of logic device beyond mainstream silicon-based Complementary Metal-Oxide Semiconductor (Si/CMOS) technology.

In FY 2012, there also are a number of significant program milestones and increases in the areas of construction and Major Items of Equipment (MIE) projects. These efforts aim at ensuring that the BES-supported scientific tools and instrumentation stay at the technological forefront and continue to charter new paths for scientific pursuits.

- The Linac Coherent Light Source (LCLS) at SLAC National Accelerator Laboratory completed construction in FY 2010 within budget, ahead of schedule, and with capabilities meeting—and in some aspects exceeding—the designed technical specifications. The LCLS is the world’s first hard X-ray free electron laser (FEL) and produces ultrafast pulses of X-rays millions of times brighter than even the most powerful synchrotron light sources. It provides scientists with a unique tool for studying the arrangement and motion of atoms and electrons in metals, semiconductors, ceramics, polymers, catalysts, plastics, and biological molecules with the potential to significantly impact advanced energy research and other fields. Capitalizing on LCLS’s success, a new MIE project for LCLS expansion (LCLS-II) is initiated in FY 2012 (+$30,000,000) to extend the x-ray spectral range at the LCLS and expand the experimentation capacity to accommodate the fast growing number of users. The LCLS-II MIE will enable the U.S. maintain leadership in FEL science and keep pace with facilities under construction elsewhere in the world.
- Support is continued for construction and Other Project Costs (FY 2012 funding of $151,400,000 and $7,700,000, respectively) for the National Synchrotron Light Source-II (NSLS-II)—built as a

replacement for NSLS—to enable the study of material properties and functions, particularly materials at the nanoscale, at a level of detail and precision never before possible. The NSLS-II project provides funding for six experimental beamlines, which is only a fraction of the total capacity. Although some of the equipment can be reused from the NSLS instruments, in order to make full use of the scientific capabilities of the new machine, new state of the art instruments need to be designed, constructed, and commissioned. A new MIE, the NSLS-II Experimental Tools (NEXT), is requested in FY 2012 (+$12,000,000) to initiate the fabrication of approximately five to six additional instruments.

- The Advanced Photon Source (APS) at Argonne National Laboratory is one of the most productive light sources in the US, serving the largest number of users per year. It is a leading machine for physical sciences, having pioneered instruments and techniques in high-pressure science, x-ray photon correlation spectroscopy and inelastic x-ray scattering. Commissioned in 1996, many of the APS components—both accelerator and instruments—were designed in the early 1990s and are not optimized for today's needs. The Advanced Photon Source Upgrade (APS-U) project is to add new x-ray capabilities and increase the number of experiments that the APS can accommodate. The new APS-U MIE project (+$20,000,000) would provide significant technical enhancements in the source's entire hard x-ray range, particularly above 20 keV, both in source brightness and intensity. Such capabilities are critically needed to examine real materials, in real time, in real environments, especially in extreme conditions encountered in advanced energy applications.
- Transmission Electron Aberration-Corrected Microscope II (TEAM II) will produce a new microscope that incorporates many of the component innovations in the initial TEAM instrument that was completed and made available to users in FY 2009. The TEAM instrument was designed with an emphasis on extending spatial resolution to new limits by fully integrating the correction of lens aberrations. The new TEAM-II MIE project (+$18,000,000) will be optimized differently to provide complementary functionality following the recommendations of a BES workshop on *Future Science Needs and Opportunities for Electron Scattering: Next-Generation Instrumentation and Beyond*. Approaches being considered include: dramatic expansion of the range of in-situ conditions (temperatures, pressures, electromagnetic fields, fluid environments) under which materials can be studied, challenges of examining soft (such as polymeric and biological or biomimetic) materials and hard/soft interfaces, and improved temporal resolution for observation of dynamic processes. These capabilities will be especially critical for exploring the unit processes and phenomena involved in clean energy technologies.
- Funding (+$47,000,000) is requested to upgrade, enhance, and procure beamlines and instruments at light sources, neutron sources, and nanoscale science research centers. The funding will be competed amongst BES scientific user facilities with the goal of significantly advancing the synthesis and characterization capabilities for clean energy technologies. This may include capabilities to collect data at high or low extremes of temperature, at high pressure, in the presence of gasses or liquid, and/or at operating voltages in a working device; to engage in materials synthesis, including high throughput combinatorial synthesis for nanoscale materials discovery and design; and for the facilities to handle full scale devices, ranging from a solar panel to a battery that powers an electric vehicle. This supports one of the key priority research directions of the BESAC Science for Energy Technology report, in which "at scale" experiments on commercial materials/devices in real-world environments is highlighted as a key enabling cross-cutting capability.

Annual Performance Results and Targets

The Department is in the process of updating its strategic plan, and has been actively engaging stakeholders including Congress. The draft strategic plan is being released for public comment concurrent with this budget submission, with the expectation of official publication this spring. The draft plan and FY 2012 budget are consistent and aligned. Updated measures will be released at a later date and available at the following link http://www.mbe.doe.gov/budget/12budget.

Materials Sciences and Engineering

Funding Schedule by Activity

	(dollars in thousands)	
	FY 2010 Current Appropriation	FY 2012 Request
Materials Sciences and Engineering		
Materials Sciences and Engineering Research	353,423	447,583
SBIR/STTR	0	12,369
Total, Materials Sciences and Engineering	353,423	459,952

Description

This subprogram supports fundamental experimental and theoretical research to provide the knowledge base for the discovery and design of new materials with novel structures, functions, and properties.

Condensed matter and materials physics research includes activities in experimental condensed matter physics, theoretical condensed matter physics, materials behavior and radiation effects, and physical behavior of materials. The research goals are supported to understand, design, and control materials properties and function. These are achieved through studies of the relationships of materials structures to their electrical, optical, magnetic, surface reactivity, and mechanical properties and investigations of material response to external forces such as stress, chemical and electrochemical environments, radiation, and the proximity of surfaces and interfaces.

Scattering and instrumentation sciences research includes activities in neutron and x-ray scattering and electron and scanning microscopies. Research is supported on the fundamental interactions of photons, neutrons, and electrons with matter to understand the atomic, electronic, and magnetic structures and excitations of materials and the relationship of these structures and excitations to materials properties and behavior.

Materials discovery, design, and synthesis research includes activities in synthesis and processing science, materials chemistry, and biomolecular materials. Research is supported in the discovery and design of novel materials and the development of innovative materials synthesis and processing methods. This research is guided by applications of concepts learned from the interface among physics, chemistry, and biology and from nanoscale understanding of synthesis and structures.

Selected FY 2010 Accomplishments

- *Smallest Superconductor Discovered.* Scientists have found the world’s smallest superconductor, a chain of four pairs of organic molecules less than one nanometer wide and only 3.5 nanometers long. In normal metals, the resistance of a wire increases as the size of the wire decreases, making it very difficult to make nanoscale metal wires because the increased resistance causes the wires to heat up and eventually melt. However, superconducting materials have no electrical resistance and can carry large electrical currents without power dissipation or heat generation. In this research, the organic superconductor $(BETS)_2GaCl_4$ (where BETS is *bis*(ethylenedithio)tetraselenafulvalene) continued to be superconducting as the molecular chains decreased from 50 nm to the length of only four pairs of molecules. This finding provides the first evidence of successful fabrication of nanoscale superconducting wires, opening up a new regime for superconductivity research that could potentially impact nanoscale electronic devices and energy applications.

- *Fractional Quantum Hall Effect Discovered in Graphene.* For the first time the fractional quantum Hall effect (FQHE) was observed in graphene, a form of carbon that has attracted attention recently because of its unusual electronic properties and potential for use in nano-electronics. Graphite is a layered material made up of 1 atom thick graphene sheets. In the FQHE, electrons interact strongly and behave collectively like new particles with a fraction of the electron's charge. Previously, the FQHE was only observed in ultrapure semiconductors at temperatures near absolute zero. These experiments confirmed the FQHE in graphene up to 20 degrees above absolute zero, indicating that electron-electron interactions are much stronger in graphene than in semiconductors. These results open the door for investigations of correlated electron behavior in graphene and have implications for future applications in electronics and quantum computing.
- *Advance in Semiconductor Nanocrystal Conductivity*: Cadmium-selenide nanorods hold promise as the active material in solar energy conversion devices. Attempts to characterize the electronic transport properties of the nanorods are extremely complicated since the addition of a metal contact alters the electronic structure of the nanorod at the metal-nanorod interface. A new synthesis technique has shown a dramatic improvement in the quality of the interface as observed by a 100,000 fold increase in the electrical conductivity of individual nanorods. Solution phase chemical deposition was used to grow gold tips on the ends of cadmium-selenide nanorods. Detailed measurements revealed that the conductivity increase is due to a 75 percent reduction of the barrier to electrical conduction. This result is attributed to maintaining an unaltered electronic structure in the semiconductor at the interface with the gold tips. These findings demonstrate the critical importance of innovative fabrication methods for the next generation of nano-sized solar photovoltaic, electronic, and optoelectronic devices.
- *Computational Design, Synthesis, and Characterization of Energy Relevant Materials.* Titanium dioxide (TiO_2) is a promising material for the conversion of sunlight into electricity. It is readily available, inexpensive and non-toxic. However, its use in photovoltaics is hampered by its relatively low absorption of visible light. Recent first principles calculations suggested that doping TiO_2 with a combination of chromium and nitrogen could vastly increase its absorption of solar radiation. The effect of the dopant is to reduce the bandgap and shift strong absorption in TiO_2 from ultraviolet to visible spectra. The calculations also predicted that the doped material was thermodynamically stable and could be synthesized. The theoretical predictions were confirmed by synthesis of doped nanometer-sized TiO_2 particles followed by characterization to confirm the properties and structure. The theoretical prediction of a material followed by the subsequent synthesis and characterization provides a rapid path to the discovery of new energy relevant materials.
- *First Identification of Individual Light Atoms by Electron Microscopy***.** For the first time, individual atoms of boron, carbon, nitrogen and oxygen have been resolved, identified, and located in materials made up of multiple elements. These light elements (with low Z, atomic number) are important components in materials for energy technologies including batteries and organic solar cells. The first atom-by-atom analysis of these light elements was made possible by an aberration-corrected scanning transmission electron microscope. The technique was used to examine a monolayer of boron nitride, revealing individual atomic substitutions involving carbon and oxygen impurity atoms. Careful analysis enabled construction of a detailed map of the atomic structure, with all the atoms of the four species resolved and identified. The new level of sensitivity is made possible by Z-contrast imaging at low operating voltages that distinguishes atoms of different Z values by their different scattering power.

- *Noble Element Xenon becomes Ignoble under Pressure***.** Research showing the high pressure reactivity of otherwise inert xenon gas revolutionizes the understanding of xenon chemistry while opening up potential routes to synthesizing a new class of hydrogen storage materials. A novel compound has been discovered—$Xe(H_2)_7$—with the highest number of hydrogen molecules per molecular unit known to date. It forms at pressures of ~40,000 atmospheres and surprisingly remains stable to much higher pressures. High resolution structure of this compound reveals that the xenon atoms coalesce into pairs that are surrounded by hydrogen molecules. These experimental data show the first evidence of the weak forces that 'glue' these two elements together to form a solid—results that have attracted the attention of theorists around the world who are trying to determine the mechanisms for bonding in these novel compounds formed at high pressure.
- *New Mechanism for Design of Materials Resistant to Radiation Damage.* A new mechanism has been discovered that holds promise for reducing the damage experienced by materials in nuclear reactors by enhancing the "healing" of defects created by the exposure to energetic neutrons. Using a combination of modeling tools, the Energy Frontier Research Center for Materials under Irradiation and Mechanical Extremes examined the role of grain boundaries on damage production and defect evolution. Molecular dynamics calculations showed that the boundaries have a complex effect on damage production by reducing the number of defects remaining after the collision cascade. By examining the damaged structures at longer time scales with temperature-accelerated dynamics calculations, it was found that radiation-induced interstitial clusters of several atoms can emit from the boundary and annihilate nearby vacancies. This can take place over many atomic distances, and occurs much faster than alternative recombination mechanisms. This result may explain the increased radiation damage resistance found in nanostructured materials, which have a large number of grain boundaries, and could be used to design improved materials for reactor applications.
- *Making Silicon Solar Cells More Efficient and Less Expensive.* The Energy Frontier Research Center for Light-Material Interactions in Energy Conversion has demonstrated for the first time that the conventional light-trapping limit for solar absorbing materials can be surpassed. They have created a new type of flexible solar cell that enhances the absorption of sunlight and efficiently converts its photons into electrons using arrays of long, thin silicon wires embedded in a polymer substrate. The new silicon wire arrays are able to absorb about 85% of the photons from incident sunlight and convert between 90 and 100 percent of these into electrons. The silicon wires measure between 30 and 100 microns in length and only 1 micron in diameter. Just 2 percent of the light-capturing elements are made up of silicon wire arrays and remaining 98% is polymer, making these solar cells less expensive and easier to produce than current solar cells, potentially via a roll-to-roll manufacturing process.

Detailed Justification

(dollars in thousands)

	FY 2010 Current Appropriation	FY 2012 Request
Materials Sciences and Engineering Research	**353,423**	**447,583**
▪ **Experimental Condensed Matter Physics**	**46,621**	**58,621**

This activity supports experimental condensed matter physics emphasizing the relationship between the electronic structure and the properties of complex materials, often at the nanoscale. The focus is on systems whose behavior derives from strong correlation effects of electrons as manifested in superconducting, semi-conducting, magnetic, thermoelectric, and optical properties. Also supported is the development of new techniques and instruments for characterizing the electronic states and properties of materials under extreme conditions, such as in ultra low temperatures (millikelvin), in ultra high magnetic fields (100 Tesla), and at ultrafast time scales (femtosecond). Capital equipment is provided for scanning tunneling microscopes, electron detectors, superconducting magnets, and physical property measurement instruments.

Improving the understanding of the electronic behavior of materials on the atomistic scale is relevant to the DOE mission, as these structures offer enhanced properties and could lead to dramatic improvements in technologies for energy generation, conversion, storage, delivery, and use. Specifically, research efforts in understanding the fundamental mechanisms of superconductivity, the elementary energy conversion steps in photovoltaics, and the energetics of hydrogen storage provide the major scientific underpinnings for the respective energy technologies. This activity also supports basic research in semiconductor and spin-based electronics of interest for the next generation information technology and electronics industries.

In FY 2012, research will continue in complex and emergent behavior. The research activities will emphasize investigations of emergent behaviors that arise from the collective, cooperative behavior of individual components of a system such as atoms or electrons that lead to physical phenomena as diverse as phase transitions, high temperature superconductivity, colossal magnetoresistance, random field magnets, and spin liquids and glasses. New research will be initiated on nanomaterials and the influence of defects and interfaces on electron transport. Research would develop mechanistic understanding to push materials performance into new regimes, with potential to significantly reduce cost and enhance lifetimes. For photovoltaics, research will focus on quantitative understanding of phenomena including in situ assessments of the effects of dopants and grain boundaries on the materials' functionality (simultaneous electronic, optical, thermal, and mechanical behavior). Additional research will be initiated to improve the wavelength conversion for solid-state lighting, with emphasis on understanding the tailoring of excitation to desired wavelengths and enhanced quantum efficiencies, while extending high temperature performance and operation lifetimes. For the grid, opportunities lie in developing the next generation of superconductors by understanding votex pinning mechanisms and thermal fluctuations in a variety of promising superconducting materials, including multiband superconductors. Research will be initiated on understanding conductivity in new classes of nanomaterials and composites, considering the implications of coupling among electronic, thermal, and mechanical properties (e.g., sagging during use).

(dollars in thousands)

	FY 2010 Current Appropriation	FY 2012 Request
Theoretical Condensed Matter Physics	**29,748**	**47,248**

This activity supports theoretical condensed matter physics with emphasis on the theory, modeling, and simulation of electronic correlations. A major thrust is nanoscale science, where links between the electronic, optical, mechanical, and magnetic properties of nanostructures and their size, shape, topology, and composition are poorly understood. Other major research areas include strongly correlated electron systems, quantum transport, superconductivity, magnetism, and optics. Development of theory targeted at aiding experimental technique design and interpretation of experimental results is also emphasized. This activity supports the Computational Materials and Chemical Sciences Network, which forms collaborating teams from diverse disciplines to address the increasing complexity of many current research issues. The activity also supports large-scale computation to perform complex calculations dictated by fundamental theory or to perform complex system simulations. Capital equipment funding will be provided for items such as computer workstations and clusters.

This activity provides the fundamental knowledge required to predict the reliability and lifetime of materials for current and future energy use and conversion technologies. Specific examples include inverse design of compound semiconductors for unprecedented solar photovoltaic conversion efficiency, solid-state approaches to improving capacity and kinetics of hydrogen storage, and ion transport mechanisms for fuel cell applications.

In FY 2012, research activities will continue to focus on enhancing the understanding of the nature and origin of highly correlated states in strongly interacting systems that have spin, charge, lattice, and orbital degrees of freedom and that are often intrinsically inhomogeneous on nanometer length scales. Research will include both theoretical and computational approaches capable of interrogating systems to gain direct insight on the mechanisms that lead to cooperative behavior. As part of *Computational Materials and Chemistry by Design*, this activity includes a significant funding increase for new research efforts to design and discover new materials with targeted properties through theory, computation, and modeling software, as validated by precise experimental characterization. Emphasis will be on the development of theory and software treating multiple length and time scales to understand dynamics, charge transport, and other properties in order to design new highly correlated materials, light-weight structural materials, metamaterials, and other advanced materials for energy applications. Simulating dynamical processes is central to modeling a wide variety of phenomena relating to materials synthesis, nanoscale, and properties in extreme environments of temperature, pressure, or radiation. Development and validation of ab initio methods and software are needed for the calculation of electronic structure, transport, phase diagrams, and evolution of structure and properties during materials use and eventual failure. Integration of correlated electronic-structure methods with quantum transport models would allow research to closely couple with electronics, materials fabrication, and energy industries.

Mechanical Behavior and Radiation Effects	**17,487**	**32,487**

This activity supports basic research to understand defects in materials and their effects on the properties of strength, structure, deformation, and failure. Defect formation, growth, migration, and propagation are examined by coordinated experimental and modeling efforts over a wide range of spatial and temporal scales. Topics include deformation of ultra-fine scale materials, radiation-resistant material fundamentals, and intelligent microstructural design for increased strength, formability, and fracture resistance in energy relevant materials. The goals are to develop predictive models for the design of materials having superior mechanical properties and radiation resistance. Capital equipment funding is provided for microstructural analysis, nanoscale mechanical property measurement tools, and ion-beam processing instrumentation.

The ability to predict materials performance and reliability and to address service life extension issues is important to the DOE mission areas of robust energy storage systems; fossil, fusion, and nuclear energy conversion; radioactive waste storage; environmental cleanup; and defense. Among the key materials performance goals for these technologies are good load-bearing capacity, failure and fatigue resistance, fracture toughness and impact resistance, high-temperature strength and dimensional stability, ductility and deformability, and radiation tolerance. Since materials from large-scale nuclear reactor components to nanoscale electronic switches undergo mechanical stress and may be subjected to ionizing radiation, this activity provides the fundamental scientific underpinning to enable the advancement of high-efficiency and safe energy generation, use, and storage as well as transportation systems.

In FY 2012, core research activities will continue to focus on understanding defects in materials and their effects on the properties of strength, structure, deformation, and failure, including ultra-fine scale materials, fundamental radiation effects, and effects of interfaces. An increase in funding is requested to significantly expand research on the properties of materials under extreme environments such as the exposure to an energetic flux, chemical reactive stimulants, high temperature and pressure. The primary emphasis will be on discovering novel phenomena and materials for improved performance with superior functionality and to establish unified models to predict the mechanical and degradation behavior of solids over multiple length and time scales. Additional research will be initiated on understanding the complex interactions of radiation-induced defects with microstructure, and their effects on the functionalities of materials under extreme conditions, emphasizing those that will exist in future generation nuclear reactor environments. The research will focus on fundamental defect interactions including the effects of helium, atomistic modeling, and designing radiation-resistant materials. Materials discovery will include nanoscale design of new materials, including materials with self-healing potential to limit the impact of defects generated by extreme exposures in reactors. In situ experiments and associated atomistic modeling will develop a fundamental understanding of kinetics of the evolution of damage microstructures. This research will be coordinated among the Office of Science, Office of Nuclear Energy, and the National Nuclear Security Administration.

	FY 2010 Current Appropriation	FY 2012 Request
▪ **Physical Behavior of Materials**	**28,533**	**46,033**

This activity supports basic research on the behavior of materials in response to external stimuli, such as temperature, electromagnetic fields, chemical environments, and the proximity effects of surfaces and interfaces. Emphasis is on the relationships between performance (such as electrical, magnetic, optical, electrochemical, and thermal performance) and the microstructure and defects in the material. Included within the activity are research to establish the relationship of crystal defects to semiconducting, superconducting, and magnetic properties; phase equilibria and kinetics of reactions in materials in hostile environments; and diffusion and transport phenomena. Basic research is also supported to develop new instrumentation, including in situ experimental tools, and to probe the physical behavior in real environments encountered in energy applications. Capital equipment funding is provided for items such as physical property measurement tools that include spectroscopic and analytical instruments for chemical and electrochemical analysis.

The research supported by this activity is necessary for improving materials reliability in chemical, electrical, and electrochemical applications and for improving the ability to generate and store energy in materials. Materials in energy-relevant environments are increasingly being exposed to extreme temperatures, strong magnetic fields, and hostile chemical conditions. A detailed understanding of how materials behavior is linked to the surroundings and treatment history is critical to the understanding of corrosion, photovoltaics, fast-ion conducting electrolytes for batteries and fuel cells, novel magnetic materials for low magnetic loss power generation, magnetocaloric materials for high-efficiency refrigeration, and new materials for high-temperature gasification.

In FY 2012, this activity will support research on the fundamental science of photon-matter interactions, which is likely to play a significant role in the development of metamaterials and nano-plasmonics—materials that are expected to be extremely important for the development of technologies that enable low cost power conversion. The research will also include the search for photoconversion materials, such as polycrystalline, nanocrystalline, and organic materials to replace expensive single crystals; innovative design of interpenetrating photoconversion materials networks to improve charge separation and collection efficiency; and the development of novel processes to obtain extremely high photo-conversion efficiencies. Funding is requested for new research on power electronics, focused on developing an understanding of the influence of defects on the properties of wide bandgap semiconductors and discovery of new magnetic materials and new, high-temperature, high-breakdown-voltage dielectric materials. Additional funding is requested to support research for the *Nanoelectronics* initiative that will focus on overcoming fundamental physics limitations to develop novel innovative concepts for nanoelectronics, including investigations of novel interconnect approaches, integration of optical and electronic materials, and novel materials for quantum information systems. In addition, new research activities will support research on degradation mechanisms and the influence of impurity diffusion on the lifetime of photovoltaics. Research will focus on understanding of intermixing and diffusion across interfaces in the structures, emphasizing compound semiconductors and cadmium-based alloys. Also included in these assessments will be development of an understanding of interface inhomogeneities on the photovoltaic performance. A mechanistic understanding will evolve that will correlate transport properties with structural evolution, interface migration, and compositional changes.

This activity also includes funding for the U.S.-India Clean Energy Research Center.

	FY 2010 Current Appropriation	FY 2012 Request
▪ **Neutron and X-ray Scattering**	**40,024**	**42,524**

This activity supports basic research on the fundamental interactions of photons and neutrons with matter to achieve an understanding of the atomic, electronic, and magnetic structures and excitations of materials and the relationships of these structures and excitations to materials properties. The main emphasis is on x-ray and neutron scattering, spectroscopy, and imaging research, primarily at major BES-supported user facilities. The development and improvement of next-generation instrumentation, novel detectors, sample environments, data analysis, tools, and technology for producing polarized neutrons are key aspects of this activity. Instrumentation development and experimental research in ultrafast materials science, including research aimed at generating, manipulating, and detecting ultrashort and ultrahigh-peak-power electron, x-ray, and laser pulses to study ultrafast physical phenomena in materials, is an integral part of the portfolio. Capital equipment funding is provided for items such as detectors, monochromators, focusing mirrors, and beamline instrumentation at the facilities.

The increasing complexity of DOE mission-relevant materials such as superconductors, semiconductors, and magnets requires ever more sophisticated scattering techniques to extract useful knowledge and to develop new theories for the behavior of these materials. X-ray and neutron scattering probes are some of the primary tools for characterizing the atomic, electronic, and magnetic structures of materials. Additionally, neutrons play a key role in hydrogen research as they provide atomic- and molecular-level information on structure, diffusion, and interatomic interactions for hydrogen. They also allow access to the morphologies that govern useful properties in catalysts, membranes, proton conductors, and hydrogen storage materials. The activity is relevant to the behavior of matter in extreme environments, especially at high pressure.

In FY 2012, research will continue to support scattering research to take advantage of increased neutron and x-ray fluxes and optimized beamline optics at BES user facilities, combined with specialized instrumentation, to investigate electrochemical processes in real time. Emphasis will be on using elastic and inelastic neutron scattering to determine structure and local dynamics and on neutron reflectivity to examine electrode/electrolyte interfaces. Time-resolved measurements will be used to study phase transformation kinetics in both amorphous and crystalline phases. The new capabilities will be used to study materials under ultrahigh pressure and to identify novel phase and phenomena not accessible via ambient conditions. Continued emphasis will be placed on materials science research to take advantage of new x-ray and neutron sources to perform research designed to understand dynamic phenomena in real-time, including the physics of strongly correlated systems, spintronics, materials at extreme conditions, and nanostructured materials for energy technologies including carbon capture phenomena, nanomagnetism, and energy storage. New research will be initiated as part of *Computational Materials and Chemistry by Design* to provide targeted experimental support for the development of algorithms and software with predictive capabilities to aid the materials discovery and design. This research will take advantage of the in situ capabilities of national user facilities for neutron and x-ray scattering for research in the discovery of advanced materials for efficient photovoltaics, electrodes and electrolytes for the next generation energy storage systems, membranes for fuel cells, carbon dioxide sequestration, radiation resistant self healing materials, and better magnets. The goal will be to facilitate stronger interaction between the experiments and theory to ensure that the experimental and computational data on structure and dynamics of functional materials are available to accelerate development and enable validation of the software. In situ research can measure properties dynamically, during synthesis and use of materials in appropriate environments and operational conditions, yielding direct data for comparison to predictions.

	(dollars in thousands)	
	FY 2010 Current Appropriation	FY 2012 Request
Electron and Scanning Probe Microscopies	**29,790**	**30,290**

This activity supports basic research in condensed matter physics and materials physics using electron scattering and microscopy and scanning probe techniques. The research includes experiments and theory to understand the atomic, electronic, and magnetic structures of materials. This activity also supports the development and improvement of electron scattering and scanning probe instrumentation and techniques, including ultrafast diffraction and imaging techniques. Capital equipment funding is provided for items such as new scanning probes and electron microscopes as well as ancillary equipment including high resolution detectors.

Performance improvements for environmentally acceptable energy generation, transmission, storage, and conversion technologies likewise depend on a detailed understanding of the structural characteristics of advanced materials. Electron and scanning probe microscopies are some of the primary tools for characterizing the atomic, electronic, and magnetic structures of materials. The activity is relevant to hydrogen research through the structural determination of nanostructured materials for hydrogen storage and solar hydrogen generation.

In FY 2012, research will emphasize the development of tools that will dramatically improve spatial, time, and energy resolution to provide fundamental understanding of the electron and charge transfer processes and mechanisms by which ions interact with electrode materials. The effort will focus on studies of transient non-equilibrium nanoscale structures, including adsorbed species in both vacuum and electrochemical environments, with near-atomic spatial resolution and at the femtosecond time scale. Ultrafast electron scattering will be developed as a companion tool to ultrafast photon probes. New research under *Computational Materials and Chemistry by Design* will be initiated to utilize microscopy, especially evolving in situ, high resolution characterization of structure and charge transport in materials for next generation batteries, photovoltaics, thermoelectrics, magnetism, and superconductivity. Development of theory and software that can predictably discover materials with designed properties requires high resolution experimental data in appropriate length and time scales at relevant conditions for the validation and refinement. The wide range of electron microscopy techniques offer superior spatial resolution and chemical speciation information complementary to x-ray and neutron scattering. The joint computational and microscopy research will assess atomic level structure, analysis of composition, evaluation of interactions of critical microstructural features, transport measurements, and the evolution of these during in situ evaluation of deformation, at elevated temperature, under straining, and other environments.

Experimental Program to Stimulate Competitive Research (EPSCoR)	**21,623**	**8,520**

This activity supports basic research spanning the broad range of science and technology programs at DOE in states that have historically received relatively less Federal research funding. The EPSCoR states are shown below. The research supported by EPSCoR includes materials sciences, chemical sciences, physics, energy-relevant biological sciences, geological and environmental sciences, high energy physics, nuclear physics, fusion energy sciences, advanced computing, and the basic sciences underpinning fossil energy, nuclear energy, and energy efficiency and renewable energy.

(dollars in thousands)

The core activity interfaces with all other core activities within the Office of Science. It is also responsive to and supports the DOE mission in the areas of energy and national security and in mitigating their associated environmental impacts.

In FY 2012, efforts will continue spanning DOE missions in the Office of Science and science underpinning a number of technology programs including Fossil Energy, Nuclear Energy, and Energy Efficiency and Renewable Energy and enhancing collaboration between programs and collaboration with DOE user facilities. The FY 2012 request will continue basic research related to DOE mission areas and will enhance collaborative efforts with DOE user facilities.

The following table shows EPSCoR distribution of funds by state.

EPSCoR Distribution of Funds by State

	FY 2010 Current Appropriation	FY 2012 Request
Alabama	547	0
Alaska	2,257	0
Arkansas	0	0
Delaware	811	649
Hawaii	0	0
Idaho	540	0
Iowa	0	0
Kansas	514	0
Kentucky	650	0
Louisiana	1,444	0
Maine	0	0
Mississippi	0	0
Montana	450	0
Nebraska	555	0
Nevada	534	0
New Hampshire	700	700
New Mexico	1,345	0
North Dakota	0	0
Oklahoma	2,900	0
Puerto Rico	470	0
Rhode Island	546	0
South Carolina	0	0

(dollars in thousands)

	FY 2010 Current Appropriation	FY 2012 Request
South Dakota	2,329	0
Tennessee	1,809	0
U.S. Virgin Islands	0	0
Utah	0	0
Vermont	0	0
West Virginia	554	0
Wyoming	2,445	0
Technical Support	223	460
Other[a]	0	6,711
▪ **Synthesis and Processing Science**	**20,777**	**24,777**

This activity supports basic research for developing new techniques to synthesize materials with desired structure, properties, or behavior; to understand the physical phenomena that underpin materials synthesis such as diffusion, nucleation, and phase transitions; and to develop in situ monitoring and diagnostic capabilities. The emphasis is on the synthesis of complex thin films and nanoscale materials with atomic layer-by-layer control; preparation techniques for pristine single crystal and bulk materials with novel physical properties; understanding the contributions of the liquid and other precursor states to the processing of bulk nanoscale materials; and low energy processing techniques for large scale nanostructured materials. The focus of this activity on bulk synthesis and crystal and thin films growth via physical means is complementary to the Materials Chemistry and Biomolecular Materials activity, which emphasizes chemical and biomimetic routes to new materials synthesis and design. Capital equipment funding is provided for crystal growth apparatus, heat treatment furnaces, lasers, chemical vapor deposition and molecular beam epitaxial processing equipment, plasma and ion sources, and deposition instruments.

Synthesis and processing science is a key component in the discovery and design of a wide variety of energy relevant materials. In this regard, the activity supports DOE’s mission in the synthesis of wide bandgap semiconductors for solid state lighting; light-weight metallic alloys for efficient transportation; novel materials such as metal organic frameworks for hydrogen storage; and structural ceramics and the processing of high temperature superconductors for near zero-loss electricity transmission. The research activity aims at providing synthesis and processing capabilities to enable the manipulation of individual spin, charge, and atomic configurations in ways to probe the atomistic basis for materials properties.

In FY 2012, research will seek to develop novel design rules for synthesizing nanostructured materials and assemblies for applications including solid-state lighting, solar energy conversion, and electrical energy storage. Research on advanced materials for electrical energy storage will include

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[a] Uncommitted funds in FY 2011, and FY 2012 will be competed among all EPSCoR states.

studies on the fundamental electrochemical characteristics of nanoscale building blocks with varying size and shape and in confined geometry. The development of new capabilities for synthesis will be emphasized including novel crystal growth techniques that will expand our ability to discover needed materials for advanced energy technologies, as well as to facilitate our understanding of new phenomena in energy generation and transport, including superconductivity, photovoltaics, and energy storage. In addition, new synthesis methods would be studied to manipulate microstructures (e.g., tailored nanoparticle dispersions) that allow enhancement of the dielectric properties of insulators and of the mechanical strength of conductors, thereby increasing the power that can be safely transmitted in the grid. Novel approaches would also be studied to create materials with increased functionality such as magnetism, but that rely on a reduced level of rare-earth additives, by understanding and controlling morphology, composition, and interfaces to understand their effects on macroscopic properties. Materials discovery research will focus on development of new materials that do not depend on rare earth additions for the desired properties.

- **Materials Chemistry and Biomolecular Materials** **57,063** **65,063**

This activity supports basic research in chemical and bio-inspired synthesis and discovery of new materials. In the materials chemistry area, discovery, design, and synthesis of novel materials with an emphasis on the chemistry and chemical control of structure and collective properties are supported. Major thrust areas include nanoscale chemical synthesis and assembly; solid state chemistry for exploratory synthesis and tailored reactivities; novel polymeric materials; surface and interfacial chemistry including electrochemistry; and the development of new, science-driven, laboratory-based analytical tools and techniques. In the biomolecular materials area, research supported includes biomimetic and bioinspired functional materials and complex structures, and materials aspects of energy conversion processes based on principles and concepts of biology. The focus on exploratory chemical and biomolecular formation of new materials is complementary to the emphasis on bulk synthesis, crystal growth, and thin films in the Synthesis and Processing Science activity. Capital equipment funding is provided for items such as advanced nuclear magnetic resonance and magnetic resonance imaging instruments and novel scanning probe microscopes.

Research supported in this activity underpins many energy-related technological areas such as batteries and fuel cells, catalysis, energy conversion and storage, friction and lubrication, high-efficiency electronic devices, hydrogen generation and storage, light-emitting materials, light-weight high-strength materials, and membranes for advanced separations.

In FY 2012, the emphasis will focus on developing a predictive understanding of the role of interfaces in the processes underpinning energy storage, photochemical, and catalytic technologies, devising experimental strategies for atom-by-atom synthesis or molecular assembly of structures, and exploring novel concepts for enhanced performance. The research will seek to advance the ability for materials to self-repair, regulate, clean, sequester impurities, and tolerate abuse. Bio-inspired materials discovery—linking physical and chemical synthesis with the synthesis strategies of biology—will be a focus to create new materials *in vitro* with altered morphologies and desired materials properties. Biological self-assembly occurs on both spatial and temporal scales and can be reversible, resulting in complex structures that are far from equilibrium, opening new avenues to materials with emergent behaviors. Additional funding will support new research to understand carbon capture phenomena, including investigation of novel chemical and biomimetic approaches for efficient carbon capture and release with a focus on kinetics and environments that include contaminants found in flue gases. Another priority area for new funding is development of improved understanding of the mechanisms responsible for system losses in organic light emitting diodes (OLEDs) and, based on this understanding, design and identification of new, novel materials with improved performance. The focus would be on research to elucidate the mechanisms for molecular interactions among the layered structures, connectors, interfaces, impurities, contacts, and their environments in high excitation conditions. A critical aspect of life extension is discerning how to limit degradation of the molecular structure due to the collision and annihilation of higher energy (blue) excitons.

	FY 2010 Current Appropriation	FY 2012 Request
▪ **Energy Frontier Research Centers (EFRCs)**[a]	**58,000**	**58,000**

The EFRCs established in late FY 2009 are multi-investigator and multi-disciplinary centers that foster, encourage, and accelerate basic research to provide the basis for transformative energy technologies of the future.[b] The EFRCs represent an important research modality for BES, bringing together the skills and talents of a critical mass of investigators to enable energy relevant, basic research of a scope and complexity that would not be possible with standard single-investigator or small-group awards. The scope and unique nature of the EFRC program requires special oversight, which is accomplished through a BES-wide, dedicated EFRC management team. This team has the direct management responsibility over all EFRCs and also coordinates EFRC research with the complementary research conducted within the BES core research areas.

This activity supports those EFRCs that are best coordinated with and most suitably complement the ongoing core research activities within the Materials Science and Engineering subprogram. These EFRCs are focused on the design, discovery, synthesis, and characterization of novel, solid-state materials that improve the conversion of solar energy and heat into electricity; that improve the conversion of electricity to light; that can be used to improve electrical energy storage; that are resistant to corrosion, decay, or failure in extreme conditions of temperature, pressure, radiation, or chemical exposures; that take advantage of emergent phenomena, such as superconductivity, to improve energy transmission; that optimize energy flow to improve energy efficiency; and that are tailored at the atomic level for catalytic activity.

In FY 2012, existing EFRCs will continue their research toward these ends. In addition, ongoing efforts to bridge disciplines, generate new avenues of inquiry, and accelerate research within the broader community will continue via periodic all-hands meetings, joint symposia and workshops, summer schools, tool development, contractors' meetings, and interactions with BES program management. BES will provide further guidance to the EFRCs to help maximize their impact and effectiveness on the basis of peer reviews of their science to be conducted during FY 2012.

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[a] A complimentary set of EFRCs is also included in the Chemical Sciences, Geosciences, and Biosciences subprogram.

[b] 16 of the 46 EFRCs awarded were forward funded for the five-year initial award period under the American Recovery and Reinvestment Act of 2009.

(dollars in thousands)

	FY 2010 Current Appropriation	FY 2012 Request
Energy Innovation Hub-Batteries and Energy Storage	**0**	**34,020**

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. Electrical energy storage offers one of the most significant solutions to the effective use of electricity in energy management. Improved energy storage is critical for more efficient and reliable smart electric grid technologies; plug-in hybrid or all-electric vehicles in the transportation sector; and the deployment of intermittent renewable energy power sources such as solar, wind, and wave energy into the utility sector. Today's electrical energy storage approaches, such as batteries and electrochemical devices, suffer from limited energy and power capacities, lower-than-desired rates of charge and discharge, calendar and cycle life limitations, low abuse tolerance, high cost, and poor performance at high or low temperatures. These performance deficiencies adversely affect the successful use and integration of renewable, intermittent power sources such as solar, wind, and wave energy into the utility sector. These same fundamental problems have also limited broad consumer acceptance and market adaptation of hybrid and all-electric vehicles.

Recent developments in nanoscience and nanotechnology offer tantalizing clues on promising scientific directions that may enable conceptual breakthroughs. They include the abilities to synthesize novel nanoscale materials with architectures tailored for specific electrochemical performance, to characterize materials and dynamic chemical processes at the atomic and molecular level, and to simulate and predict structural and functional relationships using modern computational tools. Based on this, radically new concepts in materials design can be developed for producing storage devices with materials that are abundant and low in manufacturing cost, are capable of storing higher energy densities, have long cycle lifetimes, and have high safety and abuse tolerance.

Together, these new capabilities provide the potential for addressing the gaps in cost and performance separating the current electrical energy storage technologies and those required for sustainable utility and transportation needs.

Fundamental performance limitations of energy storage systems are rooted in the constituent materials making up an electrical energy storage device, and novel approaches are needed to develop multifunctional electrical energy storage materials that offer new self-healing, self-regulating, failure-tolerant, impurity-sequestering, and sustainable characteristics.

Energy Innovation Hubs are composed of a large team of investigators focused on a single critical national need identified by the Department. Hubs integrate across the full spectrum of basic and applied research and development and bring to bear a sustained effort on our most challenging energy problems. This Hub will address a number of specific areas of energy storage research that were identified in the BES workshop report *Basic Research Needs for Electrical Energy Storage*. These include:

- Efficacy of structure in energy storage—new approaches combining theory and synthesis for the design and optimization of materials architectures including self-healing, self-regulation, failure-tolerance, and impurity sequestration.

(dollars in thousands)

	FY 2010 Current Appropriation	FY 2012 Request

- Charge transfer and transport—molecular scale understanding of interfacial electron transfer.
- Electrolytes—electrolytes with strong ionic solvation, yet weak ion-ion interactions, high fluidity, and controlled reactivity.
- Probes of energy storage chemistry and physics at all time and length scales—analytical tools capable of monitoring changes in structure and composition at interfaces and in bulk phases with spatial resolution from atomic to mesoscopic levels and temporal resolution down to femtoseconds.
- Multi-scale modeling—computational tools with improved integration of length and time scales to understand the complex physical and chemical processes that occur in electrical energy storage processes from the molecular to system scales.

One time funding of $10,000,000 will be provided for Hub start-up needs, excluding new construction.

▪ **General Plant Projects (GPP)**	**3,757**	**0**

No funds are requested in FY 2012.

SBIR/STTR	**0**	**12,369**

In FY 2010, $8,516,000 and $1,022,000 were transferred to the SBIR and STTR programs, respectively. The FY 2012 amount shown is the estimated requirement for the continuation of the congressionally mandated SBIR and STTR programs.

Total, Materials Sciences and Engineering	**353,423**	**459,952**

Explanation of Funding Changes

	FY 2012 vs. FY 2010 Current Approp. ($000)
Materials Sciences and Engineering Research	
▪ **Experimental Condensed Matter Physics**	
Increase funding for research on electron transport phenomena in materials for photovoltaics, solid state lighting, and integration of renewable technologies in the grid.	+12,000
▪ **Theoretical Condensed Matter Physics**	
Increased funding will support research for Computational Materials and Chemistry by Design for accurate design and discovery of new materials with desired functionality based on theoretical understanding using experimentally validated software.	+17,500

	FY 2012 vs. FY 2010 Current Approp. ($000)
▪ **Mechanical Behavior and Radiation Effects**	
Increased funding for enhanced research on the discovery of new materials and enhancement of the properties of materials used in extreme environments such as the exposure to an energetic neutron flux, chemical reactive stimulants, and high temperature and pressure.	+15,000
▪ **Physical Behavior of Materials**	
Increased funding for enhanced research on the fundamental science of defect physics and new materials to improve power electronics (+$3,500). Increased funding is provided for research on fundamental physics underpinning innovative concepts for nanoelectronics (+$10,000). Increased funding is requested for research on degradation, mechanisms, and impurity diffusion for photovoltaics (+$4,000).	+17,500
▪ **Neutron and X-ray Scattering**	
Increase funding will support in situ scattering research to validate computational models and software for the design of materials.	+2,500
▪ **Electron and Scanning Probe Microscopies**	
Increased funding will support utilization of microscopy and spectroscopy to validate computational methods for the design of materials.	+500
▪ **Experimental Program to Stimulate Competitive Research (EPSCoR)**	
Decrease to the FY 2010 requested level.	-13,103
▪ **Synthesis and Processing Science**	
Increased funding will support research to discover new materials for grid applications.	+4,000
▪ **Materials Chemistry and Biomolecular Materials**	
Increased funding will support research on novel materials and chemistries for carbon capture, critical research to prevent environmental carbon dioxide levels from growing to unacceptably high concentrations (+$4,000) and research to understand mechanism underlying system losses in organic light emitting diodes (+$4,000).	+8,000
▪ **Energy Innovation Hub – Batteries and Energy Storage**	
Funding is provided for the Batteries and Energy Storage Hub, to be coordinated with other DOE research and development activities for energy storage.	+34,020
▪ **GPP**	
No funds requested in FY 2012.	-3,757
Total, Materials Sciences and Engineering Research	**+94,160**

	FY 2012 vs. FY 2010 Current Approp. ($000)
SBIR/STTR	
Funding for SBIR/STTR increases relative to FY 2010 because of two issues: 1) the mandated SBIR/STTR set-asides that were transferred out of the program in FY 2010 are included in the FY 2012 request, and 2) an increase in total operating expenses from FY 2010 to FY 2012 increases the amount of the set-aside.	+12,369
Total Funding Change, Materials Sciences and Engineering	**+106,529**

Chemical Sciences, Geosciences, and Biosciences

Funding Schedule by Activity

(dollars in thousands)

	FY 2010 Current Appropriation	FY 2012 Request
Chemical Sciences, Geosciences, and Biosciences		
Chemical Sciences, Geosciences, and Biosciences Research	287,480	384,272
SBIR/STTR	0	10,445
Total, Chemical Sciences, Geosciences, and Biosciences	287,480	394,717

Description

This subprogram supports experimental, theoretical, and computational research to provide fundamental understanding of chemical transformations and energy flow in systems relevant to DOE missions. This knowledge serves as a basis for the development of new processes for the generation, storage, and use of energy and for mitigation of the environmental impacts of energy use.

In fundamental interactions, basic research is supported in atomic, molecular, and optical sciences; gas-phase chemical physics; ultrafast chemical science; theoretical and computational chemistry; and condensed phase and interfacial molecular science. Emphasis is placed on structural and dynamical studies of atoms, molecules, and nanostructures, and the description of their interactions in full quantum detail, with the aim of providing a complete understanding of reactive chemistry in the gas phase, condensed phase, and at interfaces. Novel sources of photons, electrons, and ions are used to probe and control atomic, molecular, and nanoscale matter. Ultrafast optical and x-ray techniques are developed and used to study and direct molecular, dynamics, and chemical reactions.

In photochemistry and biochemistry, including solar photochemistry, photosynthetic systems, and physical biosciences, research is supported on the molecular mechanisms involved in the capture of light energy and its conversion into chemical and electrical energy through biological and chemical pathways. Natural photosynthetic systems are studied to create robust artificial and bio-hybrid systems that exhibit the biological traits of self assembly, regulation, and self repair. Complementary research encompasses organic and inorganic photochemistry, photo-induced electron and energy transfer, photo-electrochemistry, and molecular assemblies for artificial photosynthesis.

In chemical transformations, research themes include the characterization, control, and optimization of chemistry in many forms, including catalysis; separations and analysis; actinide chemistry; and geosciences. Catalysis science underpins the design of new catalytic methods for the clean and efficient production of fuels and chemicals and emphasizes inorganic and organic complexes; interfacial chemistry, nanostructured and supramolecular catalysts, photocatalysis and electrochemistry, and bio-inspired catalytic processes. Heavy element chemistry focuses on the spectroscopy, bonding, and reactivity of actinides and fission products. Complementary research on chemical separations focuses on the use of nanoscale membranes and the development of novel metal-adduct complexes. Chemical analysis research emphasizes laser-based and ionization techniques for molecular detection, particularly the development of chemical imaging techniques. Geosciences research covers analytical and physical geochemistry, rock-fluid interactions, and flow/transport phenomena.

Selected FY 2010 Accomplishments

- *Unpeeling an Atom from the Inside Out.* A team of scientists has explored the interaction of ultrashort, high-intensity x-ray pulses with simple atoms using the world's first x-ray free-electron laser, the Linac Coherent Light Source (LCLS) at the SLAC National Accelerator Laboratory. Understanding the fundamental interaction of ultra-intense x-ray radiation with a free atom is a critical first step towards application of the LCLS to the study of more complex material systems. The recent experiments revealed the nature of the electronic response in a neon atom exposed to LCLS x-ray pulses at various photon energies for all processes that are energetically feasible through absorption of a single x-ray photon. Because the LCLS pulse is so intense and hard x-rays interact preferentially with inner-shell electrons, the neon atom is stripped of all of its electrons, starting from the inner shell of electrons followed by the outer electrons in the valence shell, creating a novel state known as a "hollow atom." The extremely rapid ejection of inner-shell electrons causes the atom to become transparent to x-ray absorption while retaining its ability to coherently scatter x-rays. This result is particularly promising for the future study of single biomolecules and nanoscale objects using the LCLS, since the techniques for imaging these objects rely on minimizing x-ray absorption (a key source of sample damage) while maximizing coherent scattering (the source of signal fidelity).
- *Nanoscale Chemical Imaging.* Chemical imaging refers to analytical and microscopy techniques that use molecular spectroscopy and often temporal resolution to obtain images of chemically distinct species at nanoscale resolution. A team of scientists has obtained images of individual zinc oxide (ZnO) nanowires, which are proposed for solar energy conversion applications, by combining atomic force microscopy with near-field scanning optical microscopy. By concentrating laser excitation light on a sharp metal tip of a scanning probe microscope, images of the chemical modifications of the ZnO surface with a spatial resolution of 100 nm were recorded. Characterization of the chemistry in such a small domain is unprecedented and important because it can reveal the influence of local variation in the sample. This new technique adds to our arsenal of chemically selective imaging techniques that are needed for the characterization of chemical processes for solar energy conversion, electrical energy storage, and catalysis.
- *Catalysts for Making Biodiesel with High Efficiency and Less Waste.* Current industrial processes for the production of biodiesel use reactions between bio-oil feedstocks and methanol that are catalyzed by sodium or potassium hydroxide. These produce the desired fatty acid esters (biodiesel) and byproducts such as glycerol and soaps. Separation of the biodiesel from the byproducts requires neutralization of the un-reacted hydroxides by strong acids, removal and disposal of toxic and corrosive chemicals, and prodigious amounts of water. This post-treatment creates waste and contributes significantly to production costs. Researchers have recently developed heterogeneous catalysts that have high activity, are easily separated from the reaction mixture by filtration, are reusable, and do not require presence of strong bases, so the overall process cost is greatly reduced and waste is reduced. In the new catalysts, silicon is substituted for calcium in calcium oxide within the porous catalytic structure. By controlling the calcium to silicon ratio, the researchers can tune reactivity to optimize biodiesel production. These catalysts were first tested successfully in a pilot plant and have now been implemented in two industrial-scale biodiesel production plants.
- *Earth-abundant Catalysts for Solar Fuel Generation.* Generation of solar fuels on a scale needed to meet global fuel demands requires that water is used as an electron source to power subsequent fuel-formation reactions. To be viable in real systems, reaction catalysts must also be robust and made from earth-abundant materials. Both cobalt and manganese oxide-based catalysts are used by nature

to drive water splitting reactions in natural photosynthesis, but catalysts of similar activity had not been developed for use in inorganic systems prior to this work. Two new oxygen-evolving electrocatalysts have been developed based on embedding earth-abundant nanoparticles of cobalt or manganese oxide in mesoporous silica structures. The particles are arranged in vertical layers in the transparent silica to efficiently utilize incident sunlight even at maximum solar intensity. In laboratory tests, the new catalysts readily produce oxygen when illuminated by sunlight and remain stable in aqueous systems. The development of effective oxygen-evolving catalysts from earth-abundant materials is a critical step toward sustainable solar fuel generation.

- *Imaging Mineral Reactivity with X-rays.* The mineral-fluid interface is the principal site of low-temperature geochemical processes at and near the Earth's surface, and therefore exerts a powerful influence on natural geochemical cycles and the response of those cycles to man-made alterations. For example, the dissolution of silicate minerals is a process that buffers atmospheric CO_2. Researchers have developed a new capability to image interfacial reactivity using x-ray microscopy at the nanometer scale. This opens up the potential for real-time imaging of the chemistry of interfacial processes as it occurs and complements physical imaging approaches such as atomic force microscopy. The research explored the effect of elevated salinity, which is the amount of dissolved salt in groundwater, on the dissolution of the mineral feldspar. *In-situ* x-ray reflectivity measurements show that increased salinity greatly increases the overall dissolution rate and leads to a rougher surface than at lower salinities. Detailed images of the reacted surfaces show that inhomogeneous dissolution leads to micron-scale regions with locally increased roughness, which provides information on the lateral variation of mineral reactivity with potential impact on understanding soil and groundwater chemistry and their interactions with atmospheric gases like CO_2.
- *A Protein that Protects Photosynthetic Apparatus Critical to Algal Survival.* Plants and algae use photosynthesis to capture solar energy and convert it into a chemical form that can be used by the cell. Too much sunlight, however, can harm photosynthetic organisms, causing severe oxidative damage and even cell death. To protect themselves, both plants and algae have evolved an energy-quenching mechanism that releases excess light energy as heat and protects the photosynthetic apparatus from damage. Researchers recently found that an evolutionarily ancient light harvesting protein, called LHSCR, was critical for survival of the green algae *Chlamydomonas reinhardtii* in a fluctuating light environment. The research suggests that this single protein in algae may play a role in both dissipating excess energy from chlorophyll and in sensing light to turn off the dissipation mechanism at the appropriate time. In higher plants, however, one protein in the light harvesting complex dissipates the energy while a different protein acts as the light sensor. The study of LHSCR in algae presents an alternative view of how nature controls solar energy harvesting and provides new insight for the effective use of algae as a biofuels feedstock and for the design of artificial light harvesting complexes.
- *Enhancing the Efficiency of Organic Photovoltaics.* Large-scale penetration of photovoltaics (PV) into the commercial electricity sector requires the development of new PV materials that have improved conversion efficiency and lower production cost than silicon. While materials based on molecular and polymer building blocks have enormous potential for being cost effective, the demonstrated conversion efficiency of these materials is ten times smaller than that of silicon. Recently, two Energy Frontier Research Centers have collaborated to develop new morphologies for organic PV materials that optimally blend interpenetrating bilayers of organic dye molecules and functionalized fullerene-like molecules to achieve a conversion efficiency of 4.1%, a significant increase over the typical 2.7% efficiencies for such materials. Researchers were guided by optical

spectroscopy and microscopy that characterized the rate of charge migration in these materials, which critically determines their conversion efficiency, and found that during the film deposition process rough, disordered interfaces with specific concentration ratios yielded the optimal morphology. The flexible modification of the morphology of these materials offers great promise for their development into cheap and efficient organic photovoltaics.

Detailed Justification

(dollars in thousands)

	FY 2010 Current Appropriation	FY 2012 Request
Chemical Sciences, Geosciences, and Biosciences Research	**287,480**	**384,272**
▪ **Atomic, Molecular, and Optical Science**	**23,011**	**24,011**

This activity supports theory and experiments to understand structural and dynamical properties of atoms, molecules, and nanostructures. The research emphasizes the fundamental interactions of these systems with photons and electrons to characterize and control their behavior. These efforts aim to develop accurate quantum mechanical descriptions of properties and dynamical processes of atoms, molecules, and nanoscale matter. The study of energy transfer within isolated molecules provides the foundation for understanding chemical reactivity, i.e., the process of energy transfer to ultimately make and break chemical bonds. Topics include the development and application of novel, ultrafast optical probes of matter, particularly x-ray sources; the interactions of atoms and molecules with intense electromagnetic fields; and studies of collisions and many-body cooperative interactions of atomic and molecular systems, including ultracold atomic and molecular gases. Capital equipment funding is provided for items such as lasers and optical equipment, unique ion sources or traps, position-sensitive and solid-state detectors, control and data processing electronics, and computational resources.

The knowledge and techniques produced by this activity form a science base that underpins several aspects of the DOE mission. New methods for using photons, electrons, and ions to probe matter lead to more effective use of BES synchrotron, nanoscience, and microcharacterization facilities. Similarly, the study of formation and evolution of energized states in atoms, molecules, and nanostructures provides a fundamental basis for understanding elementary processes in solar energy conversion and radiation-induced chemistry.

In FY 2012, research will emphasize the development and application of new ultrafast x-ray and optical probes of matter, including some of the first experiments to be performed on the Linac Coherent Light Source; theoretical and computational methods for the interpretation of ultrafast measurements; and the use of optical fields to control and manipulate quantum mechanical systems.

▪ **Chemical Physics Research**	**51,536**	**66,536**

This activity supports experimental and theoretical investigations in the gas phase, condensed phase, and at interfaces aimed at elucidating the molecular-scale chemical and physical properties and interactions that govern chemical reactivity, solute/solvent structure, and transport. Also supported are new opportunities to attain predictive understanding of chemical reactivity, including structural and dynamical studies that emphasize a complete understanding of reactive chemistry at full quantum detail. These approaches include the development and implementation of predictive computational modeling and simulation, incorporating advanced theory and experimental validation, for scientific discovery across multiple scales. Gas phase chemical physics research emphasizes studies of the dynamics and rates of chemical reactions at energies characteristic of combustion, the chemical and physical properties of key combustion intermediates, and development of experimental and theoretical tools. Combustion models are developed that incorporate complex chemistry with the turbulent flow and energy transport characteristics of real combustion processes. The overall aim is the development of a fundamental understanding of chemical reactivity enabling validated theories, models and computational tools for predicting rates, products, and dynamics of chemical processes involved in energy utilization by combustion devices. This activity includes support for the Combustion Research Facility (CRF), a multi-investigator research laboratory for the study of combustion science and technology. Condensed phase and interfacial molecular science research emphasizes chemical, physical, and electron-driven processes in aqueous media and at interfaces. Studies of reaction dynamics at well-characterized surfaces and clusters lead to the development of theories on the molecular origins of surface-mediated catalysis and heterogeneous chemistry. Studies of model condensed-phase systems target first-principles understandings of molecular reactivity and dynamical processes in solution and at interfaces. The approach confronts the transition from molecular-scale chemistry to collective phenomena in complex systems, such as the effects of solvation on chemical structure and reactivity. Research in computational and theoretical chemistry emphasizes integration and development of new and existing theoretical and computational approaches. Capital equipment funding is provided for items such as lasers and optical equipment, novel position-sensitive and temporal detectors, specialized vacuum chambers for gas-phase and surface experiments, spectrometers, and computational resources.

The impact of this activity on DOE missions is far reaching. The gas-phase portions contribute strongly to the DOE mission in the area of the efficient and clean combustion of fuels. The coupling of complex chemistry and turbulent flow has long challenged predictive combustion modeling. Truly predictive combustion models enable the design of new combustion devices (such as internal combustion engines, burners, and turbines) with maximum energy efficiency and minimal environmental consequences. In transportation, the changing composition of fuels, from those derived from light, sweet crude oil to biofuels and fuels from alternative fossil feedstocks, puts increasing emphasis on the need for science-based design of modern engines. The condensed-phase and interfacial portions impact a variety of mission areas by providing a fundamental basis for understanding chemical reactivity in complex systems, such as those encountered in catalysis and environmental processes, along with activity that provides fundamental underpinnings relevant to energy production and storage. Surface-mediated chemistry research in this activity complements more directed efforts in heterogeneous catalysis. Condensed-phase and interfacial chemical physics research on dissolution, solvation, nucleation, separation, and reaction provides important fundamental knowledge relevant to the environmental contaminant transport in mineral and aqueous environments. Fundamental studies of reactive processes driven by radiolysis in condensed phases and at interfaces provide improved understanding of radiolysis effects in nuclear fuel and waste environments.

(dollars in thousands)

	FY 2010 Current Appropriation	FY 2012 Request

In FY 2012, research will continue to emphasize fundamental interfacial and condensed phase molecular science that underpins and complements other BES efforts in heterogeneous, rediolytic chemistry, and geosciences. Research in theoretical and computation chemistry will continue to emphasize the development and application of new approaches to treat complex chemical systems. Also in FY 2012, this activity will support a new initiative in Energy Systems Simulation – Internal Combustion Engines (ESS-ICE) in collaboration with the Vehicle Technologies Program (VTP) within the Office of Energy Efficiency and Renewable Energy. Science-based, predictive simulation of combustion was identified as the single grand challenge in the BES workshop report *Basic Research Needs for Clean and Efficient Combustion of 21st Century Transportation Fuels* (2007). In a follow-up series of focused workshops with the combustion science and technology community, with emphasis on participation by U.S. automotive and engine industries, two complementary sets of codes have been identified as critical for engine design: one for stochastic, in-cylinder engine processes and one that can reliably predict the temporal and spatial behavior of liquid fuel injection. These two topics lie on the critical path toward the transition from hardware-intensive, experience-based engine design to simulation-intensive, science-based design, which is particularly important for the economic design of high-efficiency engines that can burn a broad range of fuels (including biofuels) cleanly. The ability to accurately simulate stochastic properties will allow minimization of cycle-to-cycle variations inherent in engines and allow more rapid optimization of the overall air/fuel handling and combustion processes. The liquid fuel injection code, which would include orifice flow and cavitation, atomization, dense secondary break-up, dilute spray dynamics, and vaporization, is necessary to accurately model the fuel injection processes used by all modern engines. Delivery of these two code sets for advanced engine design requires a seamless integration of basic research, focused on fundamental understanding and model systems, and engineering development, focused on device-scale simulation and testing. BES fundamental research will stress the development and experimental validation of the target codes, including experimental and theoretical studies of the complex combustion chemistry of new fuels at the high pressures, multi-phase spray dynamics, cinematic imaging diagnostics, and benchmark numerical simulations of model combustion systems that make extensive use of Office of Science leadership class computational platforms. The complementary engineering development portion of ESS-ICE will be supported by VTP, building from the long-standing and successful collaboration in basic and applied combustion science and technology between BES and VTP.

- **Solar Photochemistry** **40,241** **52,741**

This activity supports molecular-level research on solar energy capture and conversion in the condensed phase and at interfaces. These investigations of solar photochemical energy conversion focus on the elementary steps of light absorption, electrical charge generation, and charge transport within a number of chemical systems, including those with significant nanostructured composition. Supported research areas include organic and inorganic photochemistry and photocatalysis, photoinduced electron and energy transfer in the condensed phase and across interfaces, photoelectrochemistry, and artificial assemblies for charge separation and transport that mimic natural photosynthetic systems. This activity, with its integration of physical and synthetic scientists devoted to solar photochemistry, is unique to DOE. Capital equipment funding is provided for items such as ultrafast laser systems, scanning tunneling microscopes, fast Fourier transform infrared and Raman spectrometers, and computational resources.

Solar photochemical energy conversion is an important option for generating electricity and chemical fuels and therefore plays a vital role in DOE's development of solar energy as a viable component of the nation's energy supply. Photoelectrochemistry provides an alternative to semiconductor photovoltaic cells for electricity generation from sunlight using closed, renewable energy cycles. Solar photocatalysis, achieved by coupling artificial photosynthetic systems for light harvesting and charge transport with the appropriate electrochemistry, provides a direct route to the generation of fuels such as hydrogen, methane, and complex hydrocarbons. Fundamental concepts derived from studying highly efficient excited-state charge separation and transport in molecular assemblies is also applicable to future molecular optoelectronic device development.

In FY 2012, continued emphasis will be placed on studies of semiconductor/polymer interfaces, multiple charge generation within semiconductor nanoparticles, dye-sensitized solar cells, inorganic/organic donor-acceptor molecular assemblies, and the use of nanoscale materials in solar photocatalytic generation of chemical fuels. As part of the *Computational Materials and Chemistry by Design* effort, an element of the *National Materials Initiative* with other federal agencies by the Office of Science and Technology Policy, this activity includes a significant increase for the development of software tools for the simulation of light harvesting and conversion of solar energy into electricity and chemical fuels. The complexity of the underlying science for solar energy conversion requires simultaneously developing and testing computational methods and theories. Emphasis will be placed on integration and further development of scalable methods for simulating the spatial and temporal evolution of electric excitations in molecular and nanoscale systems. While computational software exists for quantitatively determining the fundamental interactions that collectively mediate charge and energy transport, these need to be carefully woven together by scientific experts in a way that allows technically adept engineers to predict carrier transport through complex solids, liquids, polymers, and interfaces.

This activity also includes funding for the U.S.-India Clean Energy Research Center.

	FY 2010 Current Appropriation	FY 2012 Request
▪ **Photosynthetic Systems**	**17,773**	**17,773**

This activity supports fundamental research on the biological conversion of solar energy to chemically stored forms of energy. Topics of study include light harvesting, exciton transfer, charge separation, transfer of reductant to carbon dioxide, as well as the biochemistry of carbon fixation and carbon storage. Emphasized areas are those involving strong intersection between biological sciences and energy-relevant chemical sciences and physics, such as in self-assembly of nanoscale components, efficient photon capture and charge separation, predictive design of catalysts, and self-regulating/repairing systems. Capital equipment funding is provided for items such as ultrafast lasers, high-speed detectors, spectrometers, environmentally controlled chambers, high-throughput robotic systems, and computational resources.

The impact of research in this activity is to uncover the underlying structure-function relationships and to probe dynamical processes in natural photosynthetic systems to guide the development of robust artificial and bio-hybrid systems for conversion of solar energy into electricity or chemical fuels. The ultimate goal is the development of bio-hybrid systems in which the best features from nature are selectively used while the shortcomings of biology are bypassed. Achieving this goal would impact DOE's efforts to develop solar energy as an efficient, renewable energy source.

In FY 2012, research will emphasize understanding and control of the weak intermolecular forces governing molecular assembly in photosynthetic systems; understanding the biological machinery for cofactor insertion into proteins and protein subunit assemblies; adapting combinatorial, directed-evolution, and high-throughput screening methods to enhance fuel production in photosynthetic systems; characterizing the structural and mechanistic features of new photosynthetic complexes; and determining the physical and chemical rules that underlie biological mechanisms of repair and photo-protection.

- **Physical Biosciences** **17,076** **17,076**

This activity combines experimental and computational tools from the physical sciences with biochemistry and molecular biology. A fundamental understanding of the complex processes that convert and store energy in living systems is sought. Research supported includes studies that investigate the mechanisms by which energy transduction systems are assembled and maintained, the processes that regulate energy-relevant chemical reactions within the cell, the underlying biochemical and biophysical principles determining the architecture of biopolymers and the plant cell wall, and active site protein chemistry that provides a basis for highly selective and efficient bio-inspired catalysts. Capital equipment is provided for items including advanced atomic force and optical microscopes, lasers and detectors, equipment for x-ray or neutron structure determinations, and Fourier transform infrared and nuclear magnetic resonance spectrometers.

The research provides basic structure-function information necessary to accomplish solid-phase nanoscale synthesis in a targeted manner, i.e., controlling the basic architecture of energy-transduction and storage systems. This impacts numerous DOE interests, including improved biochemical pathways for biofuel production, next generation energy conversion/storage devices, and efficient, environmentally benign, sustainable catalysts.

In FY 2012, continued emphasis will be placed on probing the organizational principles of biological energy transduction and chemical storage systems using advanced molecular imaging and x-ray or neutron methods for structural determination. Of particular interest is the molecular scale characterization of the structure and chemistry of the biopolymers of the plant cell wall, knowledge that is required for the direct catalytic conversion of biomass into chemical fuels.

- **Catalysis Science** **44,787** **53,787**

This activity develops the fundamental scientific principles enabling rational catalyst design and chemical transformation control. Research includes the identification of the elementary steps of catalytic reaction mechanisms and their kinetics; construction of catalytic sites at the atomic level; synthesis of ligands, metal clusters, and bio-inspired reaction centers designed to tune molecular-level catalytic activity and selectivity; the study of structure-reactivity relationships of inorganic, organic, or hybrid catalytic materials in solution or supported on solids; the dynamics of catalyst structure relevant to catalyst stability; the experimental determination of potential energy landscapes for catalytic reactions; the development of novel spectroscopic techniques and structural probes for in situ characterization of catalytic processes; and the development of theory, modeling, and simulation of catalytic pathways. Capital equipment funding is provided for items such as ultrahigh vacuum equipment with various probes of interfacial structure, spectroscopic analytical instrumentation, and specialized cells for in situ synchrotron-based experiments, and computational resources.

Catalytic transformations impact an enormous range of DOE mission areas. Particular emphasis is placed on catalysis relevant to the conversion and use of fossil and renewable energy resources and the creation of advanced chemicals. Catalysts are vital in the conversion of crude petroleum and biomass into clean burning fuels and materials. They control the electrocatalytic conversion of fuels into energy in fuel cells and batteries and play important roles in the photocatalytic conversion of energy into chemicals and materials. Catalysts are crucial to creating new, energy-efficient routes for the production of basic chemical feedstocks and value-added chemicals. Environmental applications of catalytic science include minimizing unwanted products and transforming toxic chemicals into benign ones, such as the transformation of chlorofluorocarbons into environmentally acceptable refrigerants.

In FY 2012, research will focus on the chemistry of inorganic, organic, and hybrid porous materials; the nanoscale self-assembly of these systems; and the integration of functional catalytic properties into nanomaterials. New strategies for design of selective catalysts for fuel production from both fossil and renewable biomass feedstocks will be explored. Increased emphasis will be placed on the use of spectroscopy and microscopy to probe both model systems in vacuum and realistic catalytic sites. Research on catalytic cycles involved in electrochemical energy storage and solar photocatalytic fuel formation will receive increased emphasis. As part of the *Computational Materials and Chemistry by Design* effort, this activity includes an increase for the development of predictive simulation tools for photo-catalytic, fuel-forming reactions—a critically important way in which catalyst discovery for artificial photosynthesis can be accelerated. As a verification and validation complement to the discovery of new catalysts through simulation, this activity also includes an increase for the development of new experimental approaches to the synthesis of materials and new methods to probe catalytic reactivity in situ.

	FY 2010 Current Appropriation	FY 2012 Request
▪ **Separations and Analysis**	**14,386**	**18,848**

This activity supports fundamental research covering a broad spectrum of separation concepts, including membrane processes, extraction under both standard and supercritical conditions, adsorption, chromatography, photodissociation, and complexation. Also supported is work to improve the sensitivity, reliability, and productivity of analytical determinations and to develop new approaches to analysis in complex, heterogeneous environments, including techniques that combine chemical selectivity and spatial resolution to achieve chemical imaging. This activity is the nation’s most significant long-term investment in the fundamental science underpinning actinide separations and mass spectrometry. The overall goal is to obtain a thorough understanding, at molecular and nanoscale dimensions, of the basic chemical and physical principles involved in separations systems and analytical tools so that their full utility can be realized. Capital equipment funding is provided for items such as lasers for use in sample ionization and chemical imaging, advanced mass spectrometers with nanoprobes, confocal microscopes for sub-diffraction limit resolution, and computational resources.

All effective chemical transformations require a medium to separate reactants from products. The separations of chemically distinct species and the related analytical determinations of their concentrations, often in complex environments and with extreme sensitivity, are relevant to many energy technologies. New separation media show tremendous potential for the efficient separation and subsequent capture of carbon dioxide in post-combustion gas streams and for the separation of oxygen from air required for oxy-combustion. Advanced separation membranes are also critical to the development of next-generation fuel cells. Measuring and separating contaminants from process streams in industry, or toxins from the environment, benefit from novel approaches to separations and increasingly sensitive chemical analysis.

In FY 2012, separations research will focus on fluid flow in nanoscale membranes and the formation of macroscopic separation systems via self-assembly of nanoscale building blocks. Chemical analysis research will emphasize the development of techniques with high spatial, temporal, and chemical resolution and simultaneous application of multiple analytical techniques. There is an increase for the development of new materials and methods for separation and capture of CO_2 from post-combustion gas streams and oxygen from air prior to oxy-combustion. New research in this area will include experimental and theoretical/computational studies of how weak intermolecular forces can be understood and controlled to achieve separations with high selectivity toward and capture of CO_2 with only modest energy requirements for subsequent release.

	FY 2010 Current Appropriation	FY 2012 Request
▪ **Heavy Element Chemistry**	**12,152**	**23,382**

This activity supports research in the chemistry of the heavy elements, including actinides and fission products. The unique molecular bonding of the heavy elements is explored using theory and experiment to elucidate electronic and molecular structures, bond strengths, and chemical reaction rates. Additional emphasis is placed on the chemical and physical properties of actinides to determine solution, interfacial, and solid-state bonding and reactivity; on determining chemical properties of the heaviest actinide and transactinide elements; and on bonding relationships among the actinides, lanthanides, and transition metals. Capital equipment funding is provided for items such as instruments used to characterize actinide materials (spectrometers, diffractometers, etc.) and equipment to handle the actinides safely in laboratories and at synchrotron light sources.

This activity represents the nation’s only comprehensive program that provides funding for basic research in actinide and fission product chemistry and is broadly relevant to the DOE mission. Knowledge of the chemical characteristics of actinide and fission-product materials under realistic conditions provides a basis for advanced fission fuel cycles and is coordinated with the more applied efforts within the Office of Nuclear Energy Fuel Cycle Research and Development Program. Fundamental understanding of the chemistry of these long-lived radioactive species is required to accurately predict and mitigate their transport and fate in environments associated with the storage of radioactive wastes.

In FY 2012, continued emphasis will be placed on bonding and reactivity studies in solutions, solids, nanoparticles, and interfaces, incorporating theory and modeling to understand, predict, and control the chemical bonding and reactivity of the heavy elements, especially under extreme conditions of temperature and radiation fields to be found in advanced nuclear energy systems. Increased study of organo-actinide chemistry may provide new insights into metal-carbon bonds with metals that have large ion sizes, f-orbital bonding, and multiple oxidation states. There is an increase for basic actinide chemistry research that is important for advanced nuclear fuel cycles with an emphasis on the complex separation chemistry addressing the multiplicity of chemical forms and oxidation states for actinides in fuels, solutions, and waste forms. The use of new characterization and computational tools, including DOE x-ray and neutron sources, nanoscale science research centers, and leadership computer platforms, will play an important enabling role in this new effort.

	FY 2010 Current Appropriation	FY 2012 Request
▪ **Geosciences Research**	**23,703**	**43,003**

This activity supports basic experimental and theoretical research in geochemistry and geophysics. Geochemical research emphasizes fundamental understanding of geochemical processes and reaction rates, focusing on aqueous solution chemistry, mineral-fluid interactions, and isotopic distributions and migration in natural systems. Geophysical research focuses on new approaches to understand the subsurface physical properties of fluids, rocks, and minerals and develops techniques for determining such properties at a distance; it seeks fundamental understanding of wave propagation physics in complex media and the fluid dynamics of complex fluids through porous and fractured subsurface rock units. Application of x-ray and neutron scattering using BES facilities plays a key role in the geochemical and geophysical studies within this activity. The activity also emphasizes incorporating physical and chemical understanding of geological processes into multiscale computational modeling. Capital equipment funding is provided for items such as x-ray and neutron scattering end stations at BES facilities for environmental samples and for augmenting experimental, field, and computational capabilities.

This activity provides the basic research in geosciences that underpins the nation’s strategy for understanding and mitigating the terrestrial impacts of energy technologies and thus is relevant to the DOE mission in several ways. It develops the fundamental understanding of geological processes relevant to geological disposal options for byproducts from multiple energy technologies. Knowledge of subsurface geochemical processes is essential to determining the fate and transport properties of harmful elements from possible nuclear or other waste releases. Geophysical imaging methods are needed to measure and monitor subsurface reservoirs for hydrocarbon production or for carbon dioxide storage resulting from large-scale carbon sequestration schemes.

In FY 2012, continued emphasis will be placed on geochemical studies and computational analysis of complex subsurface fluids and solids, including nanophases; understanding the dynamics of fluid flow, particulate transport and associated rock deformation in the deep subsurface; and developing the ability to integrate multiple data types in predictions of subsurface processes and properties. There is an increase for research to improve field-scale models of the dynamics of flow and plume migration in carbon sequestration. This will emphasize better understanding of reservoir-scale geochemistry; reactive flow and transport processes and rates;

higher resolution geophysical measurement techniques; and more accurate simulation approaches for linking geochemical processes and geophysical responses across multiple spatial scales. There is also an increase for a new effort to expand our understanding of the formation mechanisms of gas hydrates, and to understand and ultimately predict the environmental stability of hydrates at the systems level. This new hydrates effort will include simulation and experiment in areas including the intermolecular forces that govern the structure and properties of methane hydrates; multi-phase behavior of hydrate-sediment systems; and studies of methane hydrates in the natural environment.

	FY 2010 Current Appropriation	FY 2012 Request
▪ **Energy Frontier Research Centers (EFRCs)**[a]	**42,000**	**42,000**

The EFRCs established in late FY 2009 are multi-investigator and multi-disciplinary centers that foster, encourage, and accelerate basic research to provide the basis for transformative energy technologies of the future.[b] The EFRCs represent an important new research modality for BES, bringing together the skills and talents of a critical mass of investigators to enable energy relevant, basic research of a scope and complexity that would not be possible with the standard single-investigator or small-group award. The scope and unique nature of the EFRC program requires special oversight, which is accomplished through a BES-wide, dedicated EFRC management team. This team has the direct management responsibility over all EFRCs and also coordinates EFRC research with the complementary research conducted within the BES core research areas.

This activity supports those EFRCs that complement the ongoing core research activities within the Chemical Sciences, Geosciences and Biosciences subprogram. In general terms, these EFRCs are focused on the design, discovery, control, and characterization of chemical, biochemical, and geological moieties and processes for the advanced conversion of solar energy into chemical fuels; for improved electrochemical storage of energy; for the creation of next-generation biofuels via catalytic chemistry and biochemistry; for the clean and efficient combustion of advanced transportation fuels; and for science-based carbon capture and geological sequestration. Unifying themes in the research include the fundamental understanding of interfacial phenomena underlying the transport of electrons, atoms, molecules, and energy at the nanoscale and the development and application of new experimental and theoretical tools for molecular-scale understanding of complex chemical, biochemical, and geological processes.

In FY 2012, existing EFRCs will continue their research toward these ends. In addition, ongoing efforts to bridge disciplines, generate new avenues of inquiry, and accelerate research within the broader community will continue via periodic all-hands meetings, joint symposia and workshops, summer schools, tool development, contractors' meetings, and interactions with BES program management. BES will provide further guidance to the EFRCs to help maximize their impact and effectiveness on the basis of peer reviews of their science to be conducted during FY 2012.

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[a] A complementary set of EFRCs is also included in the Materials Sciences and Engineering subprogram.

[b] 16 EFRCs were forward funded for the five-year initial award period under the American Recovery and Reinvestment Act of 2009.

(dollars in thousands)

	FY 2010 Current Appropriation	FY 2012 Request
▪ **Energy Innovation Hub—Fuels from Sunlight**	**0**	**24,300**

After nearly 3 billion years of evolution, nature can effectively convert sunlight into energy-rich chemical fuels using the abundant feedstocks of water and carbon dioxide. All fuels used today to power vehicles and create electricity, whether from fossil or biomass resources, are ultimately derived from photosynthesis. While biofuels are renewable resources that avoid the environmental consequences of burning the sequestered carbon of fossil fuels, their scalability and sustainability are ongoing issues. Furthermore, the overall energy efficiency of converting sunlight to plant material and then converting biomass into fuels is low. The natural photosynthetic apparatus is a remarkable machine, but plants and photosynthetic microbes were not designed to meet human energy needs—much of the energy captured from the sun is necessarily devoted to the life processes of the plants. Imagine the potential energy benefits if we could generate fuels directly from sunlight, carbon dioxide, and water in a manner analogous to the natural system, but without the need to maintain life processes. The impact of replacing fossil fuels with fuels generated directly by sunlight would be immediate and revolutionary.

Basic research has already provided enormous advances in our understanding of the subtle and complex photochemistry associated with the natural photosynthetic system. Similar advances have occurred using inorganic photo-catalytic methods to split water or reduce carbon dioxide. Yet, we still lack sufficient knowledge to design solar fuel generation systems with the required efficiency, scalability, and sustainability for economic viability. Energy Innovation Hubs are composed of a large set of investigators focused on a single critical national need identified by the Department. Hubs integrate across the full spectrum of basic and applied research and development and bring to bear a sustained effort on our most challenging energy problems. The Fuels from Sunlight Hub is intended to integrate over the technical components and the basic research to applied engineering required to ultimately develop a commercially viable solar energy to chemical fuel conversion system.

The Joint Center for Artificial Photosynthesis (JCAP) was established in FY 2010 as the DOE Fuels from Sunlight Hub through a competitive Funding Opportunity Announcement that was open to universities, DOE laboratories, for-profit companies, and nonprofit entities. JCAP aims at developing a cost-effective way to produce fuels, as plants do, by combining sunlight, water, and carbon dioxide, and would be a transformational advance in carbon-neutral energy technology. Its long-term objective is to develop and demonstrate a manufacturable solar-fuels generator, made of naturally abundant elements, that will take sunlight, water, and carbon dioxide as inputs, and robustly produce fuel from the sun 10 times more efficiently than typical current crops. Research and development in JCAP will emphasize both discovery of new components necessary to meet this objective, including new light harvesting materials and fuel-forming catalysts, and the benchmarking and integration of these components into a viable solar-fuels system.

(dollars in thousands)

	FY 2010 Current Appropriation	FY 2012 Request

The Fuels from Sunlight Hub was initiated in FY 2010 with $22,000,000 provided through the Office of Energy Efficiency and Renewable Energy (EERE). SC/BES provided programmatic oversight for the establishment of the Fuels from Sunlight Hub, including management of the solicitation and its merit review process. In order to assess and guide the initial success of the Hub, it is subject to continuous management oversight by a dedicated Hub management team within BES. BES reviews all JCAP performance plans (space, conflict of interest, and intellectual property) and conducts monthly conference calls with JCAP to assess Hub progress. The Hub will submit formal quarterly progress reports to BES and will be subject to annual, external peer review, beginning in April 2011. BES continues to coordinate the activities of the Fuels from Sunlight Hub with the two other Energy Innovation Hubs initiated in FY 2010—Modeling and Simulation for Nuclear Reactors in the Office of Nuclear Energy and Energy Efficient Building Systems Design in EERE. In FY 2012, the Fuels from Sunlight Hub is funded at the planned annual level ($24,300,000), which will allow JCAP to function as an integrative Hub for DOE solar fuels research and to make timely progress on its objectives for the five-year award period.

▪ **General Plant Projects (GPP)**	**815**	**815**

GPP funding is provided for minor new construction, for other capital alterations and additions, and for improvements to land, buildings, and utility systems principally at the Ames Laboratory and the Combustion Research Facility at Sandia National Laboratories. Funding of this type is essential for maintaining the productivity and usefulness of Department-owned facilities and in meeting requirements for safe and reliable facilities operation. Additional GPP funding is included in the Materials Sciences and Engineering subprogram and the Scientific User Facilities subprogram. The total estimated cost of each GPP project will not exceed $10,000,000 in FY 2012.

SBIR/STTR	**0**	**10,445**

In FY 2010, $7,104,000 and $852,000 were transferred to the SBIR and STTR programs, respectively. The FY 2012 amount shown is the estimated requirements for the continuation of the congressionally mandated SBIR and STTR programs.

Total, Chemical Sciences, Geosciences, and Biosciences	**287,480**	**394,717**

Explanation of Funding Changes

	FY 2012 vs. FY 2010 Current Approp. ($000)
Chemical Sciences, Geosciences, and Biosciences Research	
▪ **Atomic, Molecular, and Optical Science**	
Increase in funding to emphasize the development and application of new ultrafast x-ray and optical probes of matter.	+1,000

	FY 2012 vs. FY 2010 Current Approp. ($000)
Chemical Physics Research Increase in funding to support the science-based Energy Systems Simulation - Internal Combustion Engines (ESS-ICE) initiative.	+15,000
Solar Photochemistry Increase in funding to support the *Computational Materials and Chemistry by Design* effort for the development of computational methods and software tools for the simulation of light harvesting and conversion of solar energy into electricity and chemical fuels.	+12,500
Catalysis Science Increase in funding to support the *Computational Materials and Chemistry by Design* effort for the development of computational methods and software tools for the simulation of photo-catalytic, fuel-forming reactions in artificial photosynthesis (+$5,000); for a complementary effort in catalytic synthesis and in situ characterization ($+2,000); and for research with focus on the chemistry of inorganic, organic, and hybrid porous materials (+$2,000).	+9,000
Separations and Analysis Increased funding is provided for the development of new materials and methods for separation and capture of CO_2 from post-combustion gas streams and oxygen from air prior to oxy-combustion (+$4,000). Increase in funding to continue research with focus on fluid flow in nanoscale membranes and the formation of macroscopic separation systems (+$3,692). Decrease in funding due to realignment of projects between Separations and Analysis and Heavy Element Chemistry (-$3,230).	+4,462
Heavy Element Chemistry Increase in funding for new research on actinide chemistry and separations relevant to advanced nuclear fuel cycles (+$8,000). Increase in funding due to realignment of projects between Heavy Element Chemistry and Separations and Analysis (+$3,230).	+11,230
Geosciences Research Increase in funding for the research on the multiscale dynamics of flow and plume migration in carbon sequestration (+$8,000); for new research on the formation mechanism and environmental stability of methane hydrates (+$10,000); and to continue research on geochemical studies and computational analysis of complex subsurface fluids and solids (+$1,300).	+19,300

	FY 2012 vs. FY 2010 Current Approp. ($000)
- **Energy Innovation Hub – Fuels from Sunlight** Full annual funding is provided for the Fuels from Sunlight Hub, which has a long-term mission to develop and demonstrate a manufacturable solar-fuels generation system.	+24,300
Total, Chemical Sciences, Geosciences and Biosciences Research	**+96,792**
SBIR/STTR	
Funding for SBIR/STTR increases relative to FY 2010 because of two issues: the mandated SBIR/STTR set-asides that were transferred out of the program in FY 2010 are included in the FY 2012 request, and an increase in total operating expenses from FY 2010 to FY 2012 increases the amount of the set-aside.	+10,445
Total Funding Change, Chemical Sciences, Geosciences, and Biosciences	**+107,237**

Scientific User Facilities

Funding Schedule by Activity

(dollars in thousands)

	FY 2010 Current Appropriation	FY 2012 Request
Scientific User Facilities		
Research	35,989	27,097
Major Items of Equipment	25,000	97,000
Facilities Operations	734,994	825,416
Other Project Costs	7,842	7,700
SBIR/STTR	0	21,718
Total, Scientific User Facilities	803,825	978,931

Description

This subprogram supports the R&D, planning, and operation of scientific user facilities for the development of novel nano-materials and for materials characterization through x-ray, neutron, and electron beam scattering; the former is accomplished through the Nanoscale Science Research Centers and the latter is accomplished through the world's largest suite of synchrotron radiation light source facilities, neutron scattering facilities, and electron-beam microcharacterization centers.

The BES-supported suite of facilities and research centers provides a unique set of analytical tools for studying the atomic structure and functions of complex materials. These facilities provide key capabilities to correlate the microscopic structure of materials with their macroscopic properties. The synchrotron light sources, producing photons largely over a very wide range of photon energies (from the infrared to hard x-rays), shed light on fundamental aspects of the physical world, investigating energy, momentum, and position using the techniques of spectroscopy, scattering, and imaging applied over various time scales. Neutron sources take advantage of the electrical neutrality and special magnetic properties of the neutron to probe atoms and molecules and their assembly into materials. Electron beam instruments provide the spatial resolution needed to observe individual nanostructures and even single atoms by exploiting the strong interactions of electrons with matter and the ability to readily focus beams of charged particles. The Nanoscale Science Research Centers provide the ability to fabricate complex nanostructures using chemical, biological, and other synthesis techniques, and to characterize, assemble, and integrate them into devices.

Annually, the BES user facilities are visited by more than 11,000 scientists and engineers in many fields of science and technology. These facilities provide unique capabilities to the scientific community and are a critical component of maintaining U.S. leadership in the physical sciences. The light sources are an outstanding example of serving users from a diverse range of disciplines, including physical and life sciences. For example, the life sciences sector of the light sources users increased from less than 10% in the 1990s to approximately 40% in 2010. Also supported are research activities leading to the improvement of today's facilities and better detectors, paving the foundation for the development of next generation facilities.

Selected FY 2010 Accomplishments

- *2009 Chemistry Nobel Prize to BES Synchrotron Facilities' Users.* The 2009 Nobel Prize in Chemistry for studies on ribosome was performed at the BES supported synchrotron radiation facilities. The ribosome works as a protein factory in all life organisms. Specifically, the ribosome translates the genetic instructions encoded by DNA into chains of amino acids that make up proteins. Synchrotron radiation facilities provide intense x-rays and advanced instruments enabling the studies of ribosome structures in great details at atomic level that unlocked the secret of how this protein factory functions.
- *Linac Coherent Light Source Ready for Operation.* In June 2010, the Linac Coherent Light Source (LCLS), the world's first hard x-ray free electron laser facility became officially operational. The completion of this fourth generation Linac-based light source is a milestone for x-ray user facilities. LCLS's unique capabilities will complement that of the storage ring-based third generation synchrotron light sources. The early science program, conducting experiments during the commissioning period, has already produced world-class high-impact results such as the study of femtosecond electronic response of atoms to ultra intense x-rays led by scientists at Argonne National Laboratory (see also the FY 2010 highlight under the Chemical, Physical Biosciences, and Geosciences Program section). The first open call for proposals for LCLS beam time attracted 107 proposals involving 672 scientists from 22 countries for the fall 2010 operation period.
- *Top-off Operation at Stanford Synchrotron Radiation Light Source Delivered High Flux Stable X-rays.* The Stanford Synchrotron Radiation Light Source has recently completed a successful upgrade, making top-off operation available to user service. The top-off operation makes frequent injection of electrons into the storage ring to maintain the storage ring current at an almost constant level while continually delivering x-rays to users at all times without interruption. Instead of having two major injections of a large number of electrons per day followed by uninterrupted ring current decay, the top-off operation mode adds small number of electrons to the storage ring every few minutes to offset the ring current decay during that same period of time. The near-constant ring current enhances the flux and brightness of the radiation while simultaneously improving the thermal stability of the machine and the beamline optics. The result is more x-ray photons with better beam quality delivered to users.
- *Bilayer Graphene Gets a Bandgap.* Graphene is the two-dimensional crystalline form of carbon whose extraordinary electron mobility and other unique features hold great promise for nanoscale electronics and photonics. But without a bandgap—the fundamental physical feature that makes semiconductor electronics possible—graphene's promise can't be realized. As with monolayer graphene, bilayer graphene also has a zero bandgap and thus behaves like a metal. But a bandgap can be introduced if an electric displacement field is applied to the two layers; the material then behaves like a semiconductor. A team of researchers from Lawrence Berkeley National Laboratory has engineered a bandgap in bilayer graphene that can be precisely controlled from 0 to 250 meV. To achieve this goal they used spectroscopic data obtained at the Advanced Light Source. Coupling this newly-discovered precision bandgap control with the known ability to independently manipulate the electronic states of graphene through electrical doping makes dual-gated bilayer graphene a remarkably flexible material for the development of novel nanoscale electronic devices.
- *Discovery of Element 117.* An international team of scientists from Russia and the United States established the existence of element 117 from decay patterns observed following the bombardment of the radioactive berkelium target with calcium ions at the JINR U400 cyclotron in Dubna, Russia. The berkelilum target was produced at the High Flux Isotope Reactor. Element 117 was the only

missing element in row seven of the periodic table. This discovery provides important tests of nuclear theories and offers the possibility of further expansion of the periodic table with accompanying scientific advancements in the physics and chemistry of heavy elements.

- *More Neutrons Delivered to More Users at Spallation Neutron Source.* The Spallation Neutron Source, the world's most intense pulse accelerator based neutron source, has continued to ramp up in both capability and capacity for users. The machine is operating at one megawatt beam power with over 90% reliability. Six instruments have entered the user program, while seven additional instruments are in commissioning and six more under construction. The number of scientific proposals submitted for SNS instruments' access has doubled for FY 2010 compared with FY 2009, with a significant increase in the number of unique users in FY 2010.
- *Instrumentation Developments Advance Atom Probe Tomography at the Shared Research Equipment (SHaRE) user facility.* A novel instrument, adding a laser-pulsed evaporation capability to a modern local electrode atom probe, now makes it possible for large-band-gap insulators to be successfully analyzed. Non-conducting ceramics, such as alumina, and geological samples, such as olivine, have been successfully analyzed, surmounting the prior requirement for electrically-conducting materials and permitting the technique to be applied to most solid materials. Furthermore, a new database-dependent approach is being developed for the quantification of atom probe tomography data. The high mass resolving power of the instrument has enabled this method to be applied to resolve and identify all the peaks in the mass spectrum without user interaction, with successful application to several alloys. This new capability extends the reach of atom probe tomography to a broader range of materials, while at the same time significantly shortening the time needed for data analysis.
- *Modification of Nanowires at Center for Nanoscale Materials (CNM) Enables Catalysis with Visible Light.* Nanowires of silver are well-developed materials that have been evaluated for use as transparent conductive electrodes for photovoltaic and other electronic devices. Now research at CNM has led to an integrated processing approach to chemically convert these nanowires to silver chloride and decorate them with gold nanoparticles, changing their properties substantially and enabling them to decompose organic molecules when subjected to illumination in the visible spectrum. Ions of iron generated in the initial conversion step are utilized to reduce gold precursors, leading to the surface deposition of gold on the converted silver chloride nanowires. Resonant absorption of visible light by the metal nanoparticles then drives photocatalysis. Accelerated decomposition of the organic molecule methylene blue was documented under white-light illumination at room temperature, raising the prospect that organic contaminants could potentially be removed from water using a film of such nanowires in sunlight or under fluorescent illumination.
- *Mix-and-Match Inorganic Nanocomposites Synthesized by Solution Processing at the Molecular Foundry.* Nanocomposites that consist of ordered particle assemblies in a solid matrix can have properties and behavior that are dramatically dependent on the relative shapes, sizes, and arrangements of the constituents. Researchers at the Molecular Foundry have designed a new solution-phase chemistry approach, based on colloidal nanoparticles and soluble precursors, that is capable of producing nanoscale rods, spheres, tetrapods, and other shapes. These units can then be used to form a range of assemblies including ordered superlattices, binary assemblies of two different sizes and/or types of nanoparticles, and vertically oriented arrays of nanorods. This approach offers considerable flexibility in controlling the component materials and morphology as compared with conventional methods for nanocomposite synthesis, such as thermal- or reaction-induced microphase separation or growth of nanoparticles within a porous matrix. The team demonstrated the generality of the method by creating nanocomposites of more than 20 different

compositions, starting from assemblies of spherical or rod-shaped nanoparticles. Tailored choices of materials and nanoparticle shapes and structural assemblies can be used to address a wide range of applications, from thermoelectric energy conversion to photovoltaic cells, nanostructured battery electrodes, and data storage devices.

- *Advances in Modeling at the Center for Nanophase Materials Sciences (CNMS) Improve Calculations of Magnetic Properties of Materials*. A team led by CNMS researchers has developed code for modeling magnetic structure that has achieved 1.84 thousand trillion calculations per second (1.84 petaflops). This exceptional performance was recognized by the 2009 ACM Gordon Bell Prize, which honors the world's highest-performing scientific computing applications. The project centers on a scalable method for ab initio computation of free energies in nanoscale systems, allowing direct and accurate calculations of the temperature above which a material loses its magnetism (the Curie temperature). The approach, known as the Wang-Landau Locally Self-consistent Multiple Scattering (WL-LSMS) method, differs from earlier efforts because it sets aside empirical models and their attendant approximations to tackle the system through first-principles calculations. It builds on a combination of two methods—the locally self-consistent multiple scattering (LSMS) and a Monte Carlo method known as Wang-Landau. The combination allows extension of the calculations to technologically relevant temperatures. The project thus contributes to the search for enhanced properties and stronger, more stable magnets, with implications for advances in areas such as magnetic storage and the development of lighter, stronger motors for electric vehicles.
- *High Brightness Beams Obtained with Low Charge Injection.* Recent studies have demonstrated that high brightness photon beams can be produced by a free electron laser from electron bunches carrying small amounts of charge. These electron bunches have extremely low charge but are of very high quality, i.e., they are well collimated and packed in ultrashort intense bunches. The bunch duration is shorter than the time it takes for an atom to move a significant distance (less than 100 femtoseconds) and resulted in high brightness photon beam that can be used to take snapshots of the atomic structure of matter, opening new exciting possibilities in the understanding of novel materials. In addition, these beams alleviate the difficulties of transporting high charge electron bunches by producing high photon brightness with smaller amounts of charge. These results have contributed greatly to the successful operation of the Linac Coherent Light Source.

Detailed Justification

(dollars in thousands)

	FY 2010 Current Appropriation	FY 2012 Request
Research	**35,989**	**27,097**
▪ **Electron-beam Microcharacterization**	**11,536**	**11,536**

This activity supports three electron-beam microcharacterization centers, which operate as user facilities, work to develop next-generation electron-beam instrumentation, and conduct corresponding research. These centers are the Electron Microscopy Center for Materials Research at Argonne National Laboratory (ANL), the National Center for Electron Microscopy at Lawrence Berkeley National Laboratory (LBNL), and the Shared Research Equipment program at Oak Ridge National Laboratory (ORNL). Operating funds are provided to enable expert scientific interaction and technical support and to administer a robust user program at these facilities, which are made available to all researchers with access determined via peer review of brief proposals. Capital equipment funding is provided for instruments such as scanning, transmission, and scanning transmission electron microscopes; atom probes and related field ion instruments; related surface characterization apparatus and scanning probe microscopes; and/or ancillary tools such as spectrometers, detectors, and advanced sample preparation equipment.

Electron scattering has key attributes that give such approaches unique advantages and make them complementary to x-ray and neutron beam techniques. These characteristics include strong interactions with matter (allowing the capture of meaningful signals from very small amounts of material, including single atoms under some circumstances) and the ability to readily focus the charged electron beams using electromagnetic lenses. The net result is unsurpassed spatial resolution and the ability to simultaneously get structural, chemical, and other types of information from subnanometer regions, allowing study of the fundamental mechanisms of catalysis, energy conversion, corrosion, charge transfer, magnetic behavior, and many other processes. All of these are fundamental to understanding and improving materials for energy applications and the associated physical characteristics and changes that govern performance.

In FY 2012, full user operations continue at all three of these facilities, which are routinely available to users during normal working hours. The Transmission Electron Aberration Corrected Microscope (TEAM) instrument at the National Center for Electron Microscopy at LBNL is available to the research community 24 hours a day. It leads the world in spatial resolution and embodies the first chromatic aberration corrector in an instrument of this kind, and thus its availability opens new frontiers in imaging of materials on the nanoscale for the broad scientific community. Further research and technique development proceeds using this and other instruments at the Electron Beam Microcharacterization Centers on high-resolution imaging, atomic scale tomography, in situ experimentation within electron microscopes, strain and segregation in individual nanostructures, and many other related topics.

	FY 2010 Current Appropriation	FY 2012 Request
▪ **Accelerator and Detector Research**	**15,561**	**15,561**

This activity supports basic research in accelerator physics and x-ray and neutron detectors. Accelerator research is the corner stone for the development of new technologies that will improve performance of light sources and neutron spallation facilities. This research will explore new areas of science and technologies that will facilitate the construction of next generation accelerator-based user facilities. Detector research is a crucial, but often overlooked, component in the optimal utilization of user facilities. This research program is investing aggressively in research leading to a new and more efficient generation of photon and neutron detectors. Research includes studies on creating, manipulating, transporting, and performing diagnostics of ultra-high brightness beam behavior from its origin at a photocathode to its travel through undulators. Studies on achieving sub-femtosecond (hundreds of attoseconds) free electron laser (FEL) pulses will also be underway. Demonstration experiments will take place in advanced FEL seeding techniques, such as echo-enhanced harmonic generation and other optical manipulation to reduce the cost and complexity of seeding harmonic generation FELs. A very high frequency laser photocathode radio frequency (RF) gun using a room temperature cavity will be developed which can influence the design of linac-based FELs with megahertz rates. An application will be funded for construction and testing of a

(dollars in thousands)

	FY 2010 Current Appropriation	FY 2012 Request

superconducting RF electron gun that has the potential to be the cornerstone of a future high average power FEL that combines peak performance and high average flux. Research will be done on timing and synchronization of RF and laser sources for seeded Long-wave UV (LUV) or x-ray FELs and efficient generations of seed radiation. Studies will continue on collective electron effects, such as micro-bunch instabilities from coherent synchrotron and edge radiation; beam bunching techniques, such as magnetic compression or velocity bunching; fast instruments to determine the structure of femtosecond electron bunches; and detectors capable of acquiring x-ray and neutron scattering data at very high collection rates.

This activity interacts with BES scientific research that employs synchrotron and neutron sources. It also coordinates with other DOE offices, especially in the funding of capabilities whose cost and complexity require shared support. Research at the Accelerator Test Facility at Brookhaven National Laboratory is jointly funded by the High Energy Physics and BES programs. There is also planned collaboration with the National Science Foundation (NSF) on energy recovery linac (ERL) research. There is a coordinated effort between DOE and NSF to facilitate x-ray detector development. There are ongoing industrial interactions through the DOE Small Business Innovation Research and Small Business Technology Transfer (SBIR/STTR) programs for the development of x-ray detectors and advanced accelerator technology.

In FY 2012, continued support will be provided to develop a superconducting RF electron gun that has the potential to achieve combined peak performance and high average flux. Research will continue on timing and synchronization of RF and laser sources for seeded LUV or x-ray FELs, and on efficient generations of seeded radiation. Support will also be given to the investigation of the dynamics of beam and FEL physics in the attosecond regime and the inherent challenges of creating, manipulating, transporting, and diagnosing ultra-high brightness electron beams to drive advanced light sources. A major aspect of the program support will be the need to develop light sources with new capabilities that are less costly and more compact.

	FY 2010 Current Appropriation	FY 2012 Request
▪ **General Plant Projects (GPP)**	**8,892**	**0**

GPP funding is provided in FY 2010 for the ORNL Guest House. The Guest House is designed to meet the needs of the guest users coming to perform research at ORNL's world class DOE scientific user facilities (SNS, CNMS, HFIR, SHaRE, etc.). No funds are requested in FY 2012.

	FY 2010 Current Appropriation	FY 2012 Request
Major Items of Equipment	**25,000**	**97,000**
▪ **Spallation Neutron Source Instrumentation I (SING I)**	**5,000**	**0**

Funding for the Spallation Neutron Source Instrumentation I (SING I) is completed. The Total Project Cost is $68,500,000.

	FY 2010 Current Appropriation	FY 2012 Request
▪ **Spallation Neutron Source Instrumentation II (SING II)**	**18,000**	**11,500**

Funds are provided to continue a Major Item of Equipment with an approved CD-2 Performance Baseline Total Project Cost of $60,000,000 to fabricate four instruments to be installed at the SNS. The instrument concepts for the project have been competitively selected using a peer review process. The project is managed by Oak Ridge National Laboratory.. The SING II instruments are in addition to the five instruments to be provided by the SING I project. The FY 2012 request supports the continued fabrication and installation of these instruments.

	FY 2010 Current Appropriation	FY 2012 Request
▪ **SNS Power Upgrade Project (PUP)**	**2,000**	**5,500**

Funds are provided for a Major Item of Equipment with a preliminary Total Project Cost range of \$89,600,000–\$96,100,000 for activities to design, build, install, and test the equipment necessary to increase the Spallation Neutron Source (SNS) proton beam energy. CD-1 was approved on January 16, 2009. In addition to the improvements in performance of instruments at the existing high power target station, this power upgrade will enable the eventual construction of a second target station. The existing facility layout and much of the existing SNS equipment was designed and built to meet the requirements of this upgrade.

The power upgrade project increases the linac beam energy from 1 GeV to 1.3 GeV. This will be accomplished by adding nine additional high beta cryomodules into the remaining nine open slots in the east end of the superconducting section of the linac. These additional cryomodule units will increase the number of high beta units from twelve to twenty one, allowing the energy to increase. The accelerator tunnel structure and cryogenic system were constructed to allow this upgrade.

FY 2012 Request supports continued engineering design of the accelerator sub-systems and project management.

	FY 2010 Current Appropriation	FY 2012 Request
▪ **Advanced Photon Source Upgrade (APS-U)**	**0**	**20,000**

The FY 2012 Request provides funds for a Major Item of Equipment with a preliminary Total Project Cost range of \$300,000,000-\$400,000,000 for activities to design, build, install, and test the equipment necessary to upgrade an existing third-generation synchrotron light source facility, the Advanced Photon Source (APS). Mission Need (CD-0) was approved on April 22, 2010. The APS is one of the Nation's most productive x-ray light source facilities, serving over 3500 users annually and providing key capabilities to enable forefront scientific research in a broad range of fields of physical and biological sciences. The APS is the only 7 GeV source in the U.S. and is only one of three in the world. There are only two international light sources in the class of the APS; these are the ESRF in France and SPring-8 in Japan. Both facilities, commissioned at about the same time as the APS, are well into campaigns of major upgrades due to aging of beamlines as well as technological advancements in accelerator science. With the ever increasing demand for higher penetration powers for probing real-world materials and applications, the higher energy "hard" x-rays ($E \geq 20$ keV) produced at APS provides unique capabilities in the arsenal needed for tackling the grand science and energy challenges of the 21st century—fulfilling a vision that humankind will develop materials and machines to satisfy our need for sustainable energy, healthy lives, and a thriving economy. The APS-U Project will provide an unprecedented combination of high-energy, high-average-brilliance, high flux, and short-pulse hard x-rays together with state-of-the-art x-ray beamline instrumentation. The APS-U's high-energy penetrating x-rays will provide a unique scientific capability directly relevant to problems in energy, the environment, new or improved materials, and biological studies. High-energy x-rays can penetrate into a wide range of realistic and/or extreme environments and allow us to image structures and processes in unprecedented detail.

(dollars in thousands)

FY 2010 Current Appropriation	FY 2012 Request

An upgraded APS would overcome the limitations at existing high-energy x-ray sources that prevent the simultaneous realization of nanometer spatial resolution and picosecond temporal resolution that is essential for probing and controlling a number of fundamental physical processes. The upgraded APS will complement the capabilities of the 4th generation light sources, which occupy different spectral, flux, and temporal range of technical specifications. The project is managed by Argonne National Laboratory.

The FY 2012 Request supports conceptual and preliminary engineering design and project management activities.

	FY 2010 Current Appropriation	FY 2012 Request
▪ **Linac Coherent Light Source II (LCLS-II)**	**0**	**30,000**

The FY 2012 Request provides funds for a Major Item of Equipment with a preliminary Total Project Cost range of $300,000,000-$400,000,000 for activities to design, build, install, and test the equipment that builds on the basic capabilities provided by LCLS, the world's first x-ray free electron laser (FEL), and exploit advances in technology and scientific understanding for significant improvements in capabilities and capacity. The LCLS was designed to support rapid extension of its capabilities and capacity, so as to remain the world's preeminent x-ray FEL facility even as new facilities around the world are constructed. The upgraded project (LCLS-II) will build upon the known characteristics of LCLS yet enable technologies for reaching into spectral regions not addressed by LCLS. It also provides unprecedented x-ray properties for combined control of spatial, temporal, and energy resolution that will enable groundbreaking research in a wide range of scientific disciplines, from advanced materials to energy and life sciences. Mission Need (CD-0) was approved on April 22, 2010. LCLS-II will provide extended spectral range for new applications in all scientific disciplines. The extension of the lower limit of the spectral range, and achievement of the ability to fine tune the x-ray energy, will create significant new scientific opportunities. For example, these upgrades will allow LCLS-II to reach energies that will reveal the chemistry of carbon, nitrogen, and oxygen underlies some of the most important processes in our world, such as photosynthesis involving catalytic reactivity between molecules containing carbon and oxygen.

U.S. leadership in FEL x-ray science will be challenged as competing foreign facilities are upgraded and come on-line in Germany and Japan in the 2011-2015 time frame. Upgrading the LCLS is an important next step for the U.S. to maintain world leadership in photon science by providing a suite of complementary facilities/tools covering the x-ray energy spectrum with diverse timing capabilities.

The FY 2012 request supports conceptual and preliminary engineering design and project management.

	FY 2010 Current Appropriation	FY 2012 Request
▪ **NSLS-II Experimental Tools (NEXT)**	**0**	**12,000**

The FY 2012 Request provides funds for a Major Item of Equipment with a preliminary Total Project Cost range of $50,000,000-$90,000,000 for activities to design, build, install, and test the equipment necessary to add beamlines to the National Synchrotron Light Source II (NSLS-II) Project. Mission Need (CD-0) was approved on May 27, 2010. The NEXT project will provide NSLS-II with complementary "best-in-class" beamlines that support the identified needs of the U.S. research community and the DOE energy mission. Implementation of this state-of-the-art instrumentation will significantly increase the scientific quality and productivity of NSLS-II. In addition, the NEXT project will enable and enhance more efficient operations of NSLS-II.

The FY 2012 Request supports conceptual and preliminary engineering design of the beamlines and project management.

	FY 2010 Current Appropriation	FY 2012 Request
▪ **Transmission Electron Aberration-Corrected Microscope II (TEAM II)**	**0**	**18,000**

Funds are provided for a Major Item of Equipment (MIE) with a preliminary Total Project Cost of $18,000,000 for the development, design, acquisition, installation, and testing of an advanced transmission electron microscope with novel environmental, dynamic, spectroscopic, and/or other capabilities. The original TEAM I instrument, completed and made available to users in FY 2009, was designed with an emphasis on extending spatial resolution to new limits by fully integrating the correction of lens aberrations, and set new records in that regard. It was intended as the first of a new generation of world-leading instruments, serving as a platform for developing additional microscopes tailored to other characterization needs. The development of such electron optical beamlines is analogous to the development of beamlines with varying functionalities at x-ray and neutron sources.

This TEAM II MIE will produce a new microscope that incorporates many of the component innovations in the initial instrument, but will be optimized differently to provide complementary functionality. The completed instrument would be incorporated in a BES user facility. Several approaches are being evaluated that would address the recommendations of a BES workshop on the topic, *Future Science Needs and Opportunities for Electron Scattering: Next-Generation Instrumentation and Beyond.* To address the scientific challenges identified there, high-priority directions include dramatic expansion of the range of in-situ conditions (temperatures, pressures, electromagnetic fields, fluid environments) under which materials can be studied, challenges of examining soft (such as polymeric and biological or biomimetic) materials and hard/soft interfaces, and improved temporal resolution for observation of dynamic processes. These capabilities will be especially critical for exploring the unit processes and phenomena involved in clean energy technologies.

The FY 2012 Request supports the design and fabrication of the TEAM II MIE.

	FY 2010 Current Appropriation	FY 2012 Request
Facilities Operations	**734,994**	**825,416**

This activity supports the operation of the BES scientific user facilities, which consist of light sources, neutron sources, nanoscience centers, and the Linac Coherent Light Source free electron laser at SLAC. These forefront research facilities require resource commitments well beyond the scope of any non-government institution and open up otherwise inaccessible facets of Nature to scientific inquiry. The BES user facilities provide open access to specialized instrumentation and expertise that enable scientific users from universities, national laboratories, and industry to carry out experiments and develop theories that could not be done at their home institutions. For approved, peer-reviewed projects, operating time is available without charge to researchers who intend to publish their results in the open literature. These large-scale user facilities—many of which were justified and built to serve a specific discipline of the physical sciences—have made significant contributions to many other fields of importance, including biology and medicine. The number of users for the synchrotron radiation sources and neutron scattering facilities are shown at the end of this subprogram description.

The FY 2012 budget request provides continued support for the operations of the BES scientific user facilities at an optimal level. The FY 2012 request includes additional funds for procurement of accelerator, beamline, and/or other capital equipment instrumentation to advance research capabilities for clean energy technologies. The expansion of capabilities to examine and characterize materials “at scale” and under a wide range of operating conditions across the suite of BES facilities supports key priority research directions of the BESAC Science for Energy Technology report.

The facility operations budget request includes operating funds, capital equipment, and accelerator and reactor improvement project (AIP) funding under $5,000,000. AIP funding will support additions and modifications to accelerator and reactor facilities. General plant project (GPP) funding is also required for minor new construction; for other capital alterations and additions; and for improvements to land, buildings, and utility systems. The total estimated cost of each GPP project will not exceed $10,000,000. Capital equipment is needed to maintain optimal operation at the facilities. Items include beam monitors, interlock systems, vacuum systems, beamline front end components, optical components, and new equipment at the NSRCs. A summary of the funding for the facilities is provided below.

	FY 2010	FY 2012
All Facilities		
Achieved Operating Hours	32,562	N/A
Planned Operating Hours	32,200	38,800
Optimal Hours	34,100	39,400
Percent of Optimal Hours	95%	98%
Unscheduled Downtime	6%	<10%
Number of Users	12,725	13,240

▪ **Synchrotron Radiation Light Sources**	**371,977**	**426,910**
Advanced Light Source, LBNL	60,119	71,000
Advanced Photon Source, ANL	128,275	145,050
National Synchrotron Light Source, BNL	39,000	40,725
Stanford Synchrotron Radiation Light Source, SLAC	33,950	42,235
Linac Coherent Light Source (LCLS), SLAC	16,633	127,900
Linac for LCLS, SLAC	94,000	0

The unique properties of synchrotron radiation include its continuous spectrum, high flux and brightness, and in the case of the Linac Coherent Light Source, high coherence, which makes it an indispensable tool in the exploration of matter. The wavelengths of the emitted photons span a range of dimensions from the atom to biological cells, thereby providing incisive probes for advanced research in a wide range of areas, including materials science, physical and chemical sciences, metrology, geosciences, environmental sciences, biosciences, medical sciences, and pharmaceutical sciences.

Researchers use a variety of experimental techniques when applying synchrotron radiation to their own problems. The fundamental parameters that we use to perceive the physical world (energy, momentum, position, and time) correspond to three broad categories of synchrotron experimental measurement techniques: spectroscopy, scattering, and imaging. By exploiting the short pulse lengths of synchrotron radiation, each technique can also be performed in a timing fashion.

In FY 2012, funds are provided to continue operations of the synchrotron radiation light sources. The budget also reflects an increase in the beamline and accelerator operations hours as well as user support at the LCLS as it ramps up its user program in its second full year of operations with four of the six instruments in full user service mode. Funding is also provided for capital equipment at the facilities for items such as beam monitors, interlock systems, vacuum transport systems, beamline front ends, optical components, and detectors. Additional funding will support beamline upgrades and instrumentation at BES light sources. The new and upgraded resources will enhance research opportunities for clean energy technologies.

	FY 2010	FY 2012
Advanced Light Source		
Achieved Operating Hours	5,843	N/A
Planned Operating Hours	5,500	5,600
Optimal Hours	5,600	5,600
Percent of Optimal Hours	104%	100%
Unscheduled Downtime	4.6%	<10%
Number of Users	2,032	2,300
Advanced Photon Source		
Achieved Operating Hours	4,925	N/A
Planned Operating Hours	5,000	5,000
Optimal Hours	5,000	5,000
Percent of Optimal Hours	98%	100%
Unscheduled Downtime	1.5%	<10%
Number of Users	3,796	3,800
National Synchrotron Light Source		
Achieved Operating Hours	5,735	N/A
Planned Operating Hours	5,300	5,400

	FY 2010	FY 2012
Optimal Hours	5,400	5,400
Percent of Optimal Hours	106%	100%
Unscheduled Downtime	4%	<10%
Number of Users	2,229	2,200
Stanford Synchrotron Radiation Light Source		
Achieved Operating Hours	4,870	N/A
Planned Operating Hours	5,300	5,400
Optimal Hours	5,400	5,400
Percent of Optimal Hours	90%	100%
Unscheduled Downtime	4.5%	<10%
Number of Users	1,436	1,400
Linac Coherent Light Source		
Achieved Operating Hours	0	N/A
Planned Operating Hours	0	5,000
Optimal Hours	0	5,000
Percent of Optimal Hours	0	100%
Unscheduled Downtime	0	<10%
Number of Users	359	450

▪ **High-Flux Neutron Sources**	**257,850**	**276,881**
High Flux Isotope Reactor, ORNL	60,000	68,291
Intense Pulsed Neutron Source, ANL	4,000	2,000
Manuel Lujan, Jr., Neutron Scattering Center, LANL	11,350	11,730
Spallation Neutron Source, ORNL	182,500	194,860

Neutrons are a unique and effective tool for probing the structure of matter. Beams of neutrons are particularly well-suited for measurement of the positions as well as the fluctuations in the positions of atomis (phonons), and the structure (position and direction) of atomic magnetic moments in solids and the excitations in their magnetic structure (spin waves). Such studies allow physicists to take measurements leading to an understanding of phenomena such as melting, magnetic order, and superconductivity in a variety of materials.

In FY 2012, funds are provided to continue optimal operations of the neutron sources, which are routinely available to users during normal operating hours. The funding will support the operations of additional beamlines that are coming online at the Spallation Neutron Source at ORNL. The Intense Pulsed Neutron Source is closed and funds are provided to complete decommissioning of the target assembly. Additional funding will support beamline upgrades and instrumentation at BES neutron sources. The new and upgraded resources will enhance research opportunities for clean energy technologies. Additional funding will also enhance SNS and HFIR operations for clean energy.

	FY 2010	FY 2012
High Flux Isotope Reactor		
Achieved Operating Hours	4,034	N/A
Planned Operating Hours	3,500	4,500
Optimal Hours	4,500	4,500
Percent of Optimal Hours	78%	100%
Unscheduled Downtime	0%	<10%
Number of Users	375	450
Manuel Lujan, Jr. Neutron Scattering Center		
Achieved Operating Hours	2,905	N /A
Planned Operating Hours	3,000	3,000
Optimal Hours	3,600	3,600
Percent of Optimal Hours	81%	83%
Unscheduled Downtime	15%	<10%
Number of Users	325	350
Spallation Neutron Source		
Achieved Operating Hours	4,250	N/A
Planned Operating Hours	4,600	4,900
Optimal Hours	4,600	4,900
Percent of Optimal Hours	92%	100%
Unscheduled Downtime	14%	<10%
Number of Users	430	750

	(dollars in thousands) FY 2010 Current Appropriation	FY 2012 Request
Nanoscale Science Research Centers (NSRCs)	**105,167**	**121,625**
Center for Nanophase Materials Sciences, ORNL	20,641	24,360
Center for Integrated Nanotechnologies, SNL/LANL	21,290	23,565
Molecular Foundry, LBNL	20,833	24,280
Center for Nanoscale Materials, ANL	21,570	24,810
Center for Functional Nanomaterials, BNL	20,833	24,610

The NSRCs are DOE's premier user centers for interdisciplinary research at the nanoscale, serving as the basis for a national program that encompasses new science, new tools, and new computing capabilities. Each center has particular expertise and capabilities in selected theme areas, such as synthesis and characterization of nanomaterials; catalysis; theory, modeling and simulation; electronic materials; nanoscale photonics; soft and biological materials; imaging and spectroscopy; and nanoscale integration. The centers are housed in recently-constructed and custom-designed laboratory buildings near one or more other major BES facilities for x-ray, neutron, or electron scattering, which complement and leverage the capabilities of the NSRCs. These laboratories contain clean rooms, nanofabrication resources, one-of-a-kind signature instruments, and other instruments not generally available except at major user facilities. These facilities are routinely made available to the research community during normal working hours.

In FY 2012 funds are provided to continue operations for the five NSRCs, which are routinely available to users during normal operating hours. Funding is also provided for capital equipment at the facilities for nanofabrication and characterization, and computer modeling. Additional funding will support instrumentation at the BES Nanoscale Science Research Centers. The new and upgraded resources will enhance research opportunities for clean energy technologies.

	FY 2010	FY 2012
Number of Users[a]		
Center for Nanophase Materials Sciences	360	380
Center for Integrated Nanotechnologies	358	380
Molecular Foundry	274	350
Center for Nanoscale Materials	470	380
Center for Functional Nanomaterials	281	350

Other Project Costs	**7,842**	**7,700**
National Synchrotron Light Source-II, BNL	2,000	7,700
Linac Coherent Light Source (LCLS), SLAC	5,842	0

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[a] Facility operating hours are not measured at user facilities that do not rely on one central machine.

	(dollars in thousands)	
	FY 2010 Current Appropriation	FY 2012 Request

Other Project Costs (OPC) are associated with line-item construction or major item of equipment projects and include all project costs that are not identified in the Total Estimated Cost. Total Estimated Cost includes project costs incurred after Critical Decision-1 such as costs associated with the acquisition of land and land rights; engineering, design, and inspection; direct and indirect construction/fabrication; and the initial equipment necessary to place the plant or installation in operation. Generally, OPC are costs incurred during the project's initiation and definition phase for planning, conceptual design, research and development, and during the execution phase for research and development, startup, and commissioning. Other Project Costs are always operating funds.

Funds are requested in FY 2012 for other project costs associated with the National Synchrotron Light Source-II, BNL.

SBIR/STTR	**0**	**21,718**

In FY 2010, $17,891,000 and $2,147,000 were transferred to the SBIR and STTR programs, respectively. The FY 2012 amount shown is the estimated requirement for the continuation of the congressionally mandated SBIR and STTR programs.

Subtotal, Scientific User Facilities	**803,825**	**978,931**

Explanation of Funding Changes

	FY 2012 vs. FY 2010 Current Approp. ($000)
Research	
General Plant Projects	
No GPP is requested in FY 2012. Funding for the ORNL Guest House project was completed in FY 2010.	-8,892
Major Items of Equipment	
Spallation Neutron Source Instrumentation I (SING I)	
Funding for the Major Item of Equipment for the Spallation Neutron Source Instrumentation I is completed by FY 2012.	-5,000
Spallation Neutron Source Instrumentation II (SING II)	
Scheduled decrease for the Major Item of Equipment for the Spallation Neutron Source Instrumentation II.	-6,500
SNS Power Upgrade Project (PUP)	
Scheduled increase for the Major Item of Equipment for the SNS Power Upgrade Project	+3,500

	FY 2012 vs. FY 2010 Current Approp. ($000)
▪ **Advanced Photon Source Upgrade (APS-U)**	
Initiate the Major Item of Equipment for the Advanced Photon Source Upgrade Project.	+20,000
▪ **Linac Coherent Light Source II (LCLS II)**	
Initiate the Major Item of Equipment for the Linac Coherent Light Source II Project.	+30,000
▪ **NSLS-II Experimental Tools (NEXT)**	
Initiate the Major Item of Equipment for the NSLS-II Experimental Tools Project.	+12,000
▪ **Transmission Electron Aberration-Corrected Microscope II (TEAM II)**	
Initiate the Major Item of Equipment for the Transmission Electron Aberration-Corrected Microscope II Project.	+18,000
Total, Major Items of Equipment	**+72,000**
Facilities Operations	
▪ **Synchrotron Radiation Light Sources**	
• Increase for the Advanced Light Source to support accelerator operations and users (+$2,881). Increase also requested to support beamline upgrades and instrumentation (+$8,000).	+10,881
• Increase for Advance Photon Source to support accelerator operations and users (+$7,775). Increase also requested to support beamline upgrades and instrumentation (+$9,000).	+16,775
• Increase for National Synchrotron Light Source to support accelerator operations and users.	+1,725
• Increase for the Stanford Synchrotron Radiation Light Source to support accelerator operations and users (+$1,285). Increase also requested to support beamline upgrades and instrumentation (+$7,000).	+8,285
• Increase for the Linac Coherent Light Source to support accelerator operations and users.	+17,267
Total, Synchrotron Radiation Light Sources	**+54,933**
▪ **High-Flux Neutron Source**	
• Increase for High Flux Isotope Reactor to support reactor operations (+$2,291). Increase also requested to support beamline upgrades (+$4,000) and enhance HFIR operations for clean energy (+$2,000).	+8,291

	FY 2012 vs. FY 2010 Current Approp. ($000)
• Planned decrease for the Intense Pulsed Neutron Source to finish decommissioning of the target assembly.	-2,000
• Increase for Manuel Lujan, Jr. Neutron Scattering Center to support target operations and users.	+380
• Increase for Spallation Neutron Source for new operating beamlines and to support operations and users (+$5,360). Increase also requested to support beamline upgrades (+4,000) and enhance SNS operations for clean energy (+$3,000).	+12,360
Total, High-Flux Neutron Sources	**+19,031**
▪ **Nanoscale Science Research Centers**	
• Increase for the Center for Nanophase Materials Sciences to support operations and users (+$719). Increase also requested to support instrumentation (+$3,000).	+3,719
• Increase also requested to support instrumentation (+$3,000). Decrease for the Center for Integrated Nanotechnologies due to one-time capital equipment funds provided in FY 2010 (-$725).	+2,275
• Increase for the Molecular Foundry to support operations and users (+$447). Increase also requested to support instrumentation (+$3,000).	+3,447
• Increase for the Center to Nanoscale Materials to support operations and users (+$240). Increase also requested to support instrumentation (+3,000).	+3,240
• Increase for the Center for Functional Nanomaterials to support operations and users (+$777). Increase also requested to support instrumentation (+$3,000).	+3,777
Total, Nanoscale Science Research Centers	**+16,458**
Total, Facilities Operations	**+90,422**
Other Project Costs	
▪ Increase for National Synchrotron Light Source-II per the project schedule.	+5,700
▪ Decrease for the Linac Coherent Light Source due to completion of project.	-5,842
Total, Other Project Costs	**-142**
SBIR/STTR	
Funding for SBIR/STTR increases relative to FY 2010 because of two issues: 1) the mandated SBIR/STTR set-asides that were transferred out of the program in FY 2010 are included in the FY 2012 request, and 2) an increase in total operating expenses from FY 2010 to FY 2012 increases the amount of the set-aside..	+21,718
Total Funding Change, Scientific User Facilities	**+175,106**

Construction

Funding Schedule by Activity

(dollars in thousands)

	FY 2010 Current Appropriation	FY 2012 Request
Construction		
National Synchrotron Light Source-II, BNL	139,000	151,400
Linac Coherent Light Source, SLAC	15,240	0
Total, Construction	154,240	151,400

Description

Experiments in support of basic research require construction of state-of-the-art facilities and/or that existing facilities be modified to meet unique research requirements. Reactors, x-ray light sources, and pulsed neutron sources are among the expensive, but necessary, facilities used. The budget for the BES program includes funding for the construction and modification of these facilities.

The new facility that is under construction—the National Synchrotron Light Source-II—continues the tradition of BES and SC providing the most advanced scientific user facilities for the nation's research community in the most cost effective way. The Linac Coherent Light Source completed Critical Decision 4, Approve Start of Operations in FY 2010. All of the BES construction projects are conceived and planned with the broad user community and, during construction, are maintained on schedule and within cost. Furthermore, the construction projects all adhere to the highest standards of safety. These facilities will provide the research community with the tools to fabricate, characterize, and develop new materials and chemical processes to advance basic and applied research across the full range of scientific and technological endeavor, including chemistry, physics, earth science, materials science, environmental science, biology, and biomedical science.

Performance will be measured by meeting the cost and timetables within 10% of the baseline in the construction project data sheet.

Detailed Justification

(dollars in thousands)

	FY 2010 Current Appropriation	FY 2012 Request
National Synchrotron Light Source-II (NSLS-II), BNL	**139,000**	**151,400**

The National Synchrotron Light Source-II (NSLS-II) will be a new synchrotron light source highly optimized to deliver ultra-high brightness and flux and exceptional beam stability. It will also provide advanced insertion devices, optics, detectors, robotics, and an initial suite of scientific instruments. Together, these will enable the study of material properties and functions with a spatial resolution of about 1 nm, an energy resolution of about 0.1 meV, and the ultra-high sensitivity required to perform spectroscopy on a single molecule. The NSLS-II project will design, build, and install the accelerator hardware, experimental apparatus, civil construction, and central facilities, including offices and laboratories required to produce a new synchrotron light source.

(dollars in thousands)

	FY 2010 Current Appropriation	FY 2012 Request

It includes a third generation storage ring, full energy injector, experimental areas, an initial suite of scientific instruments, and appropriate support equipment, all housed in a new building.

In FY 2012 construction funding will be used to continue civil construction activities and advance experimental and accelerator systems.

Additional information is provided in the construction project data sheet 07-SC-06.

Beyond the scope of the NSLS-II construction project, an instrument development program will be initiated in FY 2012 (the NSLS-II Experimental Tools [NEXT] project) to address new advanced experimental techniques that will go beyond the six initial instruments funded by the project.

Linac Coherent Light Source, SLAC	**15,240**	**0**

The Linac Coherent Light Source (LCLS) Project provides laser-like radiation in the x-ray region of the spectrum that is 10 billion times greater in peak brightness than any existing coherent x-ray light source. The LCLS Project provides the first demonstration of an x-ray free electron laser (FEL) in the 1.5-15 Angstrom range and will apply these extraordinary, high-brightness x-rays to an initial set of scientific problems described below. This is the world's first such facility. The LCLS has properties vastly exceeding those of earlier x-ray sources (both synchrotron radiation light sources and so-called table-top x-ray lasers) in three key areas: peak brightness, coherence (i.e., laser-like properties), and ultrashort pulses. The peak brightness of the LCLS is 10 billion times greater than current synchrotrons, providing 1011 x-ray photons in a pulse with duration of less than 230 femtoseconds. These characteristics of the LCLS will open new realms of scientific application in the chemical, material, and biological sciences.

In FY 2010, funds completed construction and commissioning of the final elements of the project. No FY 2012 funding is requested.

Total, Construction	**154,240**	**151,400**

Explanation of Funding Changes

	FY 2012 vs. FY 2010 Current Approp. ($000)
National Synchrotron Light Source-II (NSLS II), BNL	
Increase in funding to continue construction of the NSLS II project, as scheduled.	+12,400
Linac Coherent Light Source, SLAC	
Decrease in funding for the Linac Coherent Light Source, project complete.	-15,240
Total Funding Change, Construction	**-2,840**

Supporting Information

Operating Expenses, Capital Equipment and Construction Summary

	(dollars in thousands)	
	FY 2010 Current Appropriation	FY 2012 Request
Operating Expenses	1,321,471	1,590,408
Capital Equipment	81,324	195,227
General Plant Projects	19,363	4,065
Accelerator Improvement Projects	22,570	43,900
Construction	154,240	151,400
Total, Basic Energy Sciences	1,598,968	1,985,000

Funding Summary

	(dollars in thousands)	
	FY 2010 Current Appropriation	FY 2012 Request
Research	663,428	858,137
Scientific User Facilities Operations	734,994	825,416
Major Items of Equipment	25,000	97,000
Construction Projects (includes OPC)	162,082	159,100
Other	13,464	45,347
Total, Basic Energy Sciences	1,598,968	1,985,000

Scientific User Facility Operations

	(dollars in thousands)	
	FY 2010 Current Appropriation	FY 2012 Request
Light Source User Facilities		
Advanced Light Source, LBNL	60,119	71,000
Advanced Photon Source, ANL	128,275	145,050
National Synchrotron Light Source, BNL	39,000	40,725
Stanford Synchrotron Radiation Light Source, SLAC	33,950	42,235
Linac Coherent Light Source (LCLS), SLAC	16,633	127,900
Linac for LCLS, SLAC	94,000	0
Total, Light Sources User Facilities	371,977	426,910

	(dollars in thousands)	
	FY 2010 Current Appropriation	FY 2012 Request
Neutron Source User Facilities		
High Flux Isotope Reactor, ORNL	60,000	68,291
Intense Pulsed Neutron Source, ANL	4,000	2,000
Manuel Lujan, Jr. Neutron Scattering Center, LANL	11,350	11,730
Spallation Neutron Source, ORNL	182,500	194,860
Total, Neutron Source User Facilities	257,850	276,881
Nanoscale Science Research Center User Facilities		
Center for Nanophase Materials Sciences, ORNL	20,641	24,360
Center for Integrated Nanotechnologies, SNL/LANL	21,290	23,565
Molecular Foundry, LBNL	20,833	24,280
Center for Nanoscale Materials, ANL	21,570	24,810
Center for Functional Nanomaterials, BNL	20,833	24,610
Total, Nanoscale Science Research Center User Facilities	105,167	121,625
Total, Scientific User Facility Operations	734,994	825,416

Facilities Users and Hours

	FY 2010 Current Appropriation	FY 2012 Request
Advanced Light Source		
Achieved Operating Hours	5,843	N/A
Planned Operating Hours	5,500	5,600
Optimal Hours	5,600	5,600
Percent of Optimal Hours	104%	100%
Unscheduled Downtime	4.6%	<10%
Number of Users	2,032	2,300
Advanced Photon Source		
Achieved Operating Hours	4,925	N/A
Planned Operating Hours	5,000	5,000
Optimal Hours	5,000	5,000
Percent of Optimal Hours	98%	100%
Unscheduled Downtime	1.5%	<10%
Number of Users	3,796	3,800

	FY 2010 Current Appropriation	FY 2012 Request
National Synchrotron Light Source		
Achieved Operating Hours	5,735	N/A
Planned Operating Hours	5,300	5,400
Optimal Hours	5,400	5,400
Percent of Optimal Hours	106%	100%
Unscheduled Downtime	4%	<10%
Number of Users	2,229	2,200
Stanford Synchrotron Radiation Light Source		
Achieved Operating Hours	4,870	N/A
Planned Operating Hours	5,300	5,400
Optimal Hours	5,400	5,400
Percent of Optimal Hours	90%	100%
Unscheduled Downtime	4.5%	<10%
Number of Users	1,436	1,400
Linac Coherent Light Source		
Achieved Operating Hours	0	N/A
Planned Operating Hours	0	5,000
Optimal Hours	0	5,000
Percent of Optimal Hours	0	100%
Unscheduled Downtime	0	<10%
Number of Users	359	450
High Flux Isotope Reactor		
Achieved Operating Hours	4,034	N/A
Planned Operating Hours	3,500	4,500
Optimal Hours	4,500	4,500
Percent of Optimal Hours	90%	100%
Unscheduled Downtime	0%	<10%
Number of Users	375	450

	FY 2010 Current Appropriation	FY 2012 Request
Manuel Lujan, Jr. Neutron Scattering Center		
Achieved Operating Hours	2,905	N/A
Planned Operating Hours	3,000	3,000
Optimal Hours	3,600	3,600
Percent of Optimal Hours	81%	83%
Unscheduled Downtime	15%	<10%
Number of Users	325	350
Spallation Neutron Source		
Achieved Operating Hours	4,250	N/A
Planned Operating Hours	4,600	4,900
Optimal Hours	4,600	4,900
Percent of Optimal Hours	92%	100%
Unscheduled Downtime	14%	<10%
Number of Users	430	750
Center for Nanophase Materials Sciences[a]		
Number of Users	360	380
Center for Integrated Nanotechnologies[a]		
Number of Users	358	380
Molecular Foundry[a]		
Number of Users	274	350
Center for Nanoscale Materials[a]		
Number of Users	470	380
Center for Functional Nanomaterials[a]		
Number of Users	281	350
Total, All Facilities		
Achieved Operating Hours	32,562	N/A
Planned Operating Hours	32,200	38,800

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[a] Facility operating hours are not measured at user facilities that do not rely on one central machine.

	FY 2010 Current Appropriation	FY 2012 Request
Optimal Hours	34,100	39,400
Percent of Optimal Hours	95%	98%
Unscheduled Downtime	6%	<10%
Number of Users	12,725	13,240

Major Items of Equipment

(dollars in thousands)

	Prior Years	FY 2010 Current Approp.	FY 2011 CR	FY 2012 Request	Outyears	Total
Spallation Neutron Source Instrumentation I, ORNL						
TEC/TPC	63,100	5,000	400	0	0	68,500
Spallation Neutron Source Instrumentation II, ORNL						
TEC/TPC	13,500	18,000	17,000	11,500	0	60,000
SNS Power Upgrade Project , ORNL						
TEC/TPC	0	2,000	5,000	5,500	83,600	TBD
Advanced Photon Source Upgrade (APS-U), ANL						
TEC/TPC	0	0	0	20,000	TBD	TBD
Linac Coherent Light Source II (LCLS-II), SLAC						
TEC/TPC	0	0	0	30,000	TBD	TBD
NSLS-II Experimental Tools (NEXT)						
TEC/TPC, BNL	0	0	0	12,000	TBD	TBD
Transmission Electron Aberration-corrected Microscope II (TEAM II)						
TEC/TPC, TBD	0	0	0	18,000	0	18,000
Total, Major Items of Equipment						
TEC/TPC		25,000	22,400	97,000		

Construction Projects

(dollars in thousands)

	Prior Years	FY 2010 Current Approp.	FY 2011 CR	FY 2012 Request	Outyears	Total
07-SC-06, National Synchrotron Light Source-II, BNL						
TEC	276,000	139,000	151,600	151,400	73,200	791,200
OPC	57,800	2,000	1,500	7,700	51,800	120,800
TPC	333,800	141,000	153,100	159,100	125,000	912,000
05-R-320 Linac Coherent Light Source, SLAC						
TEC	336,760	15,240	0	0	0	352,000[a]
OPC	56,500	5,842	0	0	0	62,342[b]
TPC	393,260	21,082	0	0	0	414,342[b]
Total, Construction						
TEC		154,240	151,600	151,400		
OPC		7,842	1,500	7,700		
TPC		162,082	153,100	159,100		

Scientific Employment

	FY 2010 Actual	FY 2012 Estimate
# of University Grants	1,210	1,480
Average Size per year	175,000	200,000
# Permanent Ph.D's (FTEs)	4,670	5,700
# Postdoctoral Associates (FTEs)	1,300	1,650
# Graduate Students (FTEs)	2,050	2,600

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[a] Includes $35,974,000 of PED included in the 03-SC-002 PED, SLAC, Linac Coherent Light Source data sheet.

[b] The TPC has been reduced due to favorable performance, especially in commissioning, which allowed the project to finish one month ahead of schedule, and under the budgeted TPC of $420,000,000 for project. Remaining OPC funds were transferred to LCLS Operations.

07-SC-06, National Synchrotron Light Source II (NSLS-II)
Brookhaven National Laboratory, Upton, New York
Project Data Sheet is for PED/Construction

1. Significant Changes

The most recent DOE O 413.3B approved Critical Decision (CD) is CD-3, Start of Construction, which was approved on January 9, 2009, with a Total Project Cost (TPC) of $912,000,000. The project is approximately two years past CD-3 approval. The overall project is approximately 44% complete with cumulative project Cost Performance Index (CPI) and Schedule Performance Index (SPI) at the end of November 2010 at 1.02 and 1.00 respectively.

The Federal Project Director was certified at level 4 in September of 2010.

The project experienced some minor delays with the PED effort that necessitated delaying completion. The value of the delayed work is $286,000.

This PDS is an update of the FY 2011 PDS.

2. Design, Construction, and D&D Schedule

	CD-0	CD-1	(Design/PED Complete)	CD-2	CD-3	CD-4
FY 2007	08/25/2005	1Q FY 2007	4Q FY 2008	TBD	TBD	TBD
FY 2008	08/25/2005	2Q FY 2007	2Q FY 2009	TBD	TBD	TBD
FY 2009	08/25/2005	07/12/2007	2Q FY 2009	2Q FY 2008	2Q FY 2009	3Q FY 2015
FY 2010	08/25/2005	07/12/2007	2Q FY 2009	01/18/2008	01/09/2009	3Q FY 2015
FY 2011	08/25/2005	07/12/2007	4Q FY 2010	01/18/2008	01/09/2009	3Q FY 2015
FY 2012	08/25/2005	07/12/2007	4Q FY 2011	01/18/2008	01/09/2009	3Q FY 2015

CD-0 – Approve Mission Need
CD-1 – Approve Alternative Selection and Cost Range
CD-2 – Approve Performance Baseline
CD-3 – Approved Start of Construction
CD-4 – Approve Project Completion

	D&D Start	D&D Complete	Performance Baseline Validation
FY 2007	N/A	N/A	N/A
FY 2008	N/A	N/A	N/A
FY 2009	N/A	N/A	12/11/2007
FY 2010	N/A	N/A	12/11/2007
FY 2011	N/A	N/A	12/11/2007
FY 2012	N/A	N/A	12/11/2007

D&D Start – Not Applicable to this project
D&D Complete – Not Applicable to this project

3. Baseline and Validation Status

(dollars in thousands)

	TEC, PED	TEC, Construction	TEC, Total	OPC Except D&D	OPC D&D	OPC, Total	TPC
FY 2007	75,000	TBD	TBD	TBD	TBD	TBD	TBD
FY 2008	75,000	TBD	TBD	TBD	TBD	TBD	TBD
FY 2009	60,000	731,200	791,200	120,800	0	120,800	912,000
FY 2010	60,000	731,200	791,200	120,800	0	120,800	912,000
FY 2011	60,000	731,200	791,200	120,800	0	120,800	912,000
FY 2012	60,000	731,200	791,200	120,800	0	120,800	912,000

4. Project Description, Justification, and Scope

The National Synchrotron Light Source II (NSLS-II) will be a new synchrotron light source, highly optimized to deliver ultra-high brightness and flux and exceptional beam stability. It will also provide advanced insertion devices, optics, detectors, robotics, and an initial suite of scientific instruments. Together, these will enable the study of material properties and functions with an unprecedented combination of state-of-the-art technical specifications: spatial resolution of about 1 nm, an energy resolution of about 0.1 meV, and the ultra-high sensitivity required to perform spectroscopy on a single molecule.

The NSLS-II project will design, build, and install the accelerator hardware, experimental apparatus, civil construction, and central facilities including offices and laboratories required to produce a new synchrotron light source. It includes a third generation storage ring, full energy injector, experimental areas, an initial suite of scientific instruments, and appropriate support equipment, all housed in a new building.

Major advances in energy technologies will require scientific breakthroughs in developing new materials with advanced properties. A broad discussion is given in several recent reports, including the Basic Energy Sciences (BES) Advisory Committee reports entitled *Opportunities for Catalysis in the 21st Century*, *Basic Research Needs to Assure a Secure Energy Future*, *Basic Research Needs for the Hydrogen Economy*, and *Basic Research Needs for Solar Energy Utilization*, in addition to the report of the Nanoscale Science, Engineering, and Technology Subcommittee of the National Science and Technology Committee entitled *Nanoscience Research for Energy Needs*.

Collectively, these reports underscore the need to develop new tools that will allow the characterization of the atomic and electronic structure, the chemical composition, and the magnetic properties of materials with nanoscale resolution. Needed are non-destructive tools to image and characterize structures and interfaces below the surface, and these tools must operate in a wide range of temperature and harsh environments. The absence of any tool possessing these combined capabilities was identified as a key barrier to progress in the 1999 BES report *Nanoscale Science, Engineering and Technology Research Directions*.

In order to fill this capability gap, the Office of Science has determined that its mission requires a synchrotron light source that will enable the study of material properties and functions, particularly materials at the nanoscale, at a level of detail and precision never before possible. NSLS-II will provide these capabilities. Only x-ray methods have the potential of satisfying all of these requirements, but advances both in x-ray optics and in x-ray brightness and flux are required to achieve a spatial resolution of 1 nm and an energy resolution of 0.1 meV.

There are no alternative tools with a spatial resolution of 1 nm and energy resolution of 0.1 meV that also have the required capabilities of being non-destructive and able to image and characterize buried structures and interfaces in a wide range of temperatures and harsh environments. In the case of NSLS-I, it was found that it would be impossible to upgrade this light source due to numerous technical difficulties, including accelerator physics and infrastructure constraints, such as its small circumference, which limit the feasible in-place upgrade options.

The key performance parameters are defined in the project execution plan. The NSLS-II project is expected to deliver an electron energy of 3.0 giga-electron volts with a stored current of 25 milliamps; build a third generation storage ring of approximately one half mile in circumference and experimental and operations facilities with a total conventional construction of approximately 400 thousand gross square feet, and include an initial suite of six beamlines ready for commissioning.

Research and development activities funded under Other Project Costs will address technical risk in several key areas including energy resolution, spatial resolution, and storage ring magnets.

Beyond the scope of the NSLS-II construction project, an instrument development program has been implemented. The NSLS II Experimental Tools (NEXT) Project MIE, received CD-0 approval in May 2010 and will provide five to six state-of-the-art scientific instruments at NSLS II with a preliminary cost range of $50M to $90M.

Project Engineering and Design funds were used to complete the detailed design, including detailed estimates of construction based on the approved design, final working drawings and specifications, and schedules for construction and procurements.

The construction of the Ring Building is progressing well and as of December 2010 is 70% complete. Steel erection is completed and the roofing, siding, interior mechanical and electrical systems are well advanced. System start-up is in progress for the Ring Building, Pentant 1 where beneficial occupancy is scheduled for February 2011. The construction contract for the Laboratory Office Buildings (LOB) has been awarded and construction of foundations is underway. All other major civil construction sub-contracts, including the Electrical Substation and Central Chilled Water Facility expansion, are at or near 100% complete. Contracts to fabricate the storage ring magnets have been awarded, with first article and production magnets being delivered and tested. The Linac and the Booster contracts were also awarded. The final design review of the Linac has been completed, with the supplier working towards the building and delivery of the Linac front end. The Booster final design review will be completely shortly. Beamline technical specifications are being finalized and statements of work for long-lead procurements are being developed.

FY 2012 funds will be used to continue civil construction and advance experimental and accelerator systems.

The project is being conducted in accordance with the project management requirements in DOE Order 413.3B, Program and Project Management for the Acquisition of Capital Assets, and all appropriate project management requirements have been met.

5. Financial Schedule

(dollars in thousands)

	Appropriations	Obligations	Recovery Act Costs	Costs
Total Estimated Cost (TEC)				
PED				
FY 2007	3,000	3,000	0	2,292
FY 2008	29,727	29,727	0	28,205
FY 2009	27,273	27,273	0	23,044
FY 2010	0	0	0	6,173
FY 2011[a]	0	0	0	286
Total, PED	60,000	60,000	0	60,000
Construction				
FY 2009	66,000	66,000	0	24,092
FY 2009 Recovery Act	150,000	150,000	14,751	0
FY 2010	139,000	139,000	67,424	84,826
FY 2011[a]	151,600	151,600	59,624	205,982
FY 2012	151,400	151,400	8,201	110,611
FY 2013	46,900	46,900	0	105,995
FY 2014	26,300	26,300	0	41,230
FY 2015	0	0	0	8,464
Total, Construction	731,200	731,200	150,000	581,200
TEC				
FY 2007	3,000	3,000	0	2,292
FY 2008	29,727	29,727	0	28,205
FY 2009	93,273	93,273	0	47,136
FY 2009 Recovery Act	150,000	150,000	14,751	0
FY 2010	139,000	139,000	67,424	90,999
FY 2011[a]	151,600	151,600	59,624	206,268
FY 2012	151,400	151,400	8,201	110,611
FY 2013	46,900	46,900	0	105,995
FY 2014	26,300	26,300	0	41,230
FY 2015	0	0	0	8,464
Total, TEC	791,200	791,200	150,000	641,200

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[a] The FY 2011 amounts reflect the FY 2011 funding under the FY 2011 Continuing Resolution.

(dollars in thousands)

	Appropriations	Obligations	Recovery Act Costs	Costs
Other Project Cost (OPC)				
OPC except D&D				
FY 2005	1,000	1,000	0	0
FY 2006	4,800	4,800	0	4,958
FY 2007	22,000	22,000	0	20,461
FY 2008	20,000	20,000	0	15,508
FY 2009	10,000	10,000	0	7,101
FY 2010	2,000	2,000	0	5,852
FY 2011[a]	1,500	1,500	0	4,638
FY 2012	7,700	7,700	0	9,458
FY 2013	24,400	24,400	0	24,000
FY 2014	22,400	22,400	0	22,400
FY 2015	5,000	5,000	0	6,424
Total, OPC except D&D	120,800	120,800	0	120,800
Total Project Cost (TPC)				
FY 2005	1,000	1,000	0	0
FY 2006	4,800	4,800	0	4,958
FY 2007	25,000	25,000	0	22,753
FY 2008	49,727	49,727	0	43,713
FY 2009	103,273	103,273	0	54,237
FY 2009 Recovery Act	150,000	150,000	14,751	0
FY 2010	141,000	141,000	67,424	96,851
FY 2011[a]	153,100	153,100	59,624	210,906
FY 2012	159,100	159,100	8,201	120,069
FY 2013	71,300	71,300	0	129,995
FY 2014	48,700	48,700	0	63,630
FY 2015	5,000	5,000	0	14,888
Total, TPC	912,000	912,000	150,000	762,000

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[a] The FY 2011 amounts reflect the FY 2011 funding under the FY 2011 Continuing Resolution.

6. Details of Project Cost Estimate

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design (PED)			
Design	60,000	60,000	49,000
Contingency	0	0	11,000
Total, PED	60,000	60,000	60,000
Construction			
Site Preparation	9,243	9,243	9,243
Equipment	31,579	32,078	31,579
Other Construction	567,885	545,379	518,381
Contingency	122,493	144,500	171,997
Total, Construction	731,200	731,200	731,200
Total, TEC	791,200	791,200	791,200
Contingency, TEC	122,493	144,500	182,997
Other Project Cost (OPC)			
Conceptual Planning	24,800	24,800	24,800
Research and Development	35,800	35,800	35,800
Start-Up	50,200	50,200	50,200
Contingency	10,000	10,000	10,000
Total, OPC	120,800	120,800	120,800
Contingency, OPC	10,000	10,000	10,000
Total, TPC	912,000	912,000	912,000
Total, Contingency	132,493	154,500	192,997

7. Funding Profile History

(dollars in thousands)

Request Year		Prior Years	FY 2009	FY 2009 Recovery Act	FY 2010	FY 2011	FY 2012	FY 2013	FY 2014	FY 2015	Total
FY 2007[a]	TEC	75,000	0	0	0	0	0	0	0	0	75,000
	OPC	46,000	0	0	0	0	0	0	0	0	46,000
	TPC	121,000	0	0	0	0	0	0	0	0	121,000

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[a] The FY 2007 and FY 2008 requests were for PED funding only.

(dollars in thousands)

Request Year		Prior Years	FY 2009	FY 2009 Recovery Act	FY 2010	FY 2011	FY 2012	FY 2013	FY 2014	FY 2015	Total
FY 2008[a]	TEC	65,000	10,000	0	0	0	0	0	0	0	75,000
	OPC	50,800	0	0	0	0	0	0	0	0	50,800
	TPC	115,800	10,000	0	0	0	0	0	0	0	125,800
FY 2009[a]	TEC	32,727	93,273	0	162,500	252,900	166,100	57,400	26,300	0	791,200
	OPC	47,800	10,000	0	2,000	1,500	7,700	24,400	22,400	5,000	120,800
	TPC	80,527	103,273	0	164,500	254,400	173,800	81,800	48,700	5,000	912,000
FY 2010	TEC	32,727	93,273	150,000	139,000	151,600	151,400	46,900	26,300	0	791,200
	OPC	47,800	10,000	0	2,000	1,500	7,700	24,400	22,400	5,000	120,800
	TPC	80,527	103,273	150,000	141,000	153,100	159,100	71,300	48,700	5,000	912,000
FY 2011	TEC	32,727	93,273	150,000	139,000	151,600	151,400	46,900	26,300	0	791,200
	OPC	47,800	10,000	0	2,000	1,500	7,700	24,400	22,400	5,000	120,800
	TPC	80,527	103,273	150,000	141,000	153,100	159,100	71,300	48,700	5,000	912,000
FY 2012	TEC	32,727	93,273	150,000	139,000	151,600[b]	151,400	46,900	26,300	0	791,200
	OPC	47,800	10,000	0	2,000	1,500[b]	7,700	24,400	22,400	5,000	120,800
	TPC	80,527	103,273	150,000	141,000	153,100[b]	159,100	71,300	48,700	5,000	912,000

8. Related Operations and Maintenance Funding Requirements

Beneficial Occupancy of the Experimental Floor	4Q FY 2012
Expected Useful Life (number of years)	25
Expected Future start of D&D of this capital asset (fiscal quarter)	N/A

(Related Funding Requirements)

(dollars in thousands)

	Annual Costs		Life cycle costs	
	Current Estimate	Prior Estimate	Current Estimate	Prior Estimate
Operations	119,400	119,400	4,470,000	4,470,000
Maintenance	21,100	21,100	789,000	789,000
Total Operations and Maintenance	140,500	140,500	5,259,000	5,259,000

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[a] FY 2009 reflects the original validated funding baseline.

[b] The FY 2011amounts reflect the FY 2011 funding under the FY 2011 Continuing Resolution.

9. Required D&D Information

	Square Feet
Area of new construction	Approximately 400,000
Area of existing facilities being replaced	N/A
Area of any additional space that will require D&D to meet the "one-for-one" requirement	NA (see below)

The existing facility (NSLS) will be converted to another use. The one-for-one replacement has been met through completed and planned elimination of space at Brookhaven National Laboratory (BNL) along with "banked" space at the Massachusetts Institute of Technology (MIT) in Middleton, MA, and at the East Tennessee Technology Park (ETTP) in Oak Ridge, TN. A waiver from the one-for-one requirement to eliminate excess space at Brookhaven to offset the NSLS-II project was approved by Secretary Bodman on April 20, 2007. The waiver identified approximately 460,000 square feet of banked excess facilities space that were eliminated in FY 2006 at MIT and ETTP.

10. Acquisition Approach

The acquisition strategy selected relies on the BNL management and operating (M&O) contractor to directly manage the NSLS-II acquisition. The acquisition of large research facilities is within the scope of the DOE contract for the management and operation of BNL and consistent with the general expectation of the responsibilities of DOE M&O contractors.

The design, fabrication, assembly, installation, testing, and commissioning of the NSLS-II project will largely be performed by the BNL NSLS-II scientific and technical staff. Much of the subcontracted work to be performed for NSLS-II consists of hardware fabrication and conventional facilities construction. Each system or component will be procured using fixed price contracts, unless there is a compelling reason to employ another contract type. Best-value competitive procurements will be employed to the maximum extent possible.

Many major procurements are either build-to-print, following BNL/NSLS-II drawings and specifications, or readily available off-the-shelf. Source selection will be carried out in accordance with DOE-approved policies and procedures. Acquisition strategies have been chosen to obtain the best value based on the assessment of technical and cost risks on a case-by-case basis. For standard, build-to-print fabrications and the purchase of off-the-shelf equipment for routine applications, available purchasing techniques include price competition among technically qualified suppliers and use of competitively awarded blanket purchase agreements are used.

The architect-engineer (A-E) contract was placed on a firm-fixed-price basis for the Final (Title II) Design and (Title III) construction support services. The general construction contract was also placed on a firm-fixed-price basis. The design specifications are detailed and allow prospective constructors to formulate firm-fixed-price offers without excessive contingency and allowances.

NSLS-II project management has identified major procurements that represent significant complexity or cost and schedule risk. Advance procurement plans (APPs) are prepared for each major procurement. The APPs include discussion of contract type, special contracting methods, special clauses or deviations required, and lease or purchase decisions. These final APPs will identify critical procurement activities and help to mitigate or avoid schedule conflicts and other procurement-related problems. At appropriate dollar levels, the APPs are approved by the responsible Division Director, the NSLS-II Procurement Manager, the NSLS-II Deputy Director, the NSLS-II Project Director and the DOE Site Office.