Basic Energy Sciences

Overview

The mission of the Basic Energy Sciences (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.

The research disciplines that BES supports—condensed matter and materials physics, chemistry, geosciences, and aspects of physical biosciences—are those that discover new materials and design new chemical processes that touch virtually every important 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 helps build the foundation to achieve the vision of a secure and sustainable energy future. BES also supports world-class, open-access scientific user facilities consisting of a complementary set of intense x-ray sources, neutron sources, and research centers for nanoscale science. BES facilities probe materials with ultrahigh spatial, temporal, and energy resolutions to interrogate the critical functions of matter—transport, reactivity, fields, excitations, and motion—and answer some of the most challenging grand science questions. BES-supported activities are entering a new era in which materials can be built with atom-by-atom precision and computational models can predict the behavior of materials before they exist.

As history has shown, breakthroughs in clean energy technologies will likely be built on a foundation of basic research advances. Key to exploiting such discoveries is the ability to create new materials using sophisticated synthesis and processing techniques, precisely define the atomic arrangements in matter, and control physical and chemical transformations. The energy systems of the future—whether they tap sunlight, store electricity, or make fuel by 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.

Highlights of the FY 2015 Budget Request

In FY 2015, BES will support ongoing core research activities at approximately the FY 2014 level. A new activity on computational materials sciences is proposed that will support integrated theoretical modeling and experimental research to develop community codes and research-oriented software for predictive design of functional materials. The Energy Frontier Research Centers (EFRCs) funding will continue at the FY 2014 level, and funding for the Energy Innovation Hubs will continue as planned.

The FY 2015 budget request reflects choices between operating existing facilities, upgrading facilities, and building new user facilities. In FY 2015, BES will support the optimal operations of four light source facilities, two neutron source facilities, and five Nanoscale Science Research Centers (NSRCs). Funding will be increased to continue early operations of the National Synchrotron Light Source-II (NSLS-II) as it transitions from a construction project to operations in FY 2015. Construction funding for NSLS-II will be ramped down as the project is completed in FY 2015, as scheduled. The National Synchrotron Light Source (NSLS) will cease operations and funds are provided to transition the facility to a safe storage condition in FY 2015. The BES operations at the Lujan Neutron Scattering Center will cease and funding is requested to transition the facility to a safe storage condition. The three electron beam microcharacterization centers will be merged administratively with their respective neighboring NSRCs in FY 2015. The Advanced Photon Source Upgrade (APS-U) and the NSLS-II Experimental Tools (NEXT) major item of equipment (MIE) projects will be supported. The Linac Coherent Light Source-II (LCLS-II) construction project scope will be modified to include the addition of a superconducting linear accelerator and additional undulators to deliver an unprecedented high-repetition-rate free-electron laser that will solidify the Linac Coherent Light Source complex as the world leader in ultrafast x-ray science for a decade or more.

In FY 2015, the Chemical Transformations activity will collaborate with the Offices of Energy Efficiency and Renewable Energy, Fossil Energy, Electricity Delivery and Energy Reliability, and Nuclear Energy on a crosscutting initiative on subsurface engineering.

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Funding ($K)

	FY 2013 Current	FY 2014 Enacted	FY 2014 Current	FY 2015 Request	FY 2015 vs. FY 2014 Enacted
Materials Sciences and Engineering					
Scattering and Instrumentation Sciences Research	61,731	64,022	64,022	64,022	0
Condensed Matter and Materials Physics Research	120,946	120,946	120,946	120,946	0
Materials Discovery, Design, and Synthesis Research	73,983	73,983	73,983	73,983	0
Experimental Program to Stimulate Competitive Research (EPSCoR)	8,416	9,953	9,953	8,520	-1,433
Energy Frontier Research Centers (EFRCs)	57,320	58,000	58,000	58,000	0
Energy Innovation Hubs—Batteries and Energy Storage	24,237	24,237	24,237	24,175	-62
Computational Materials Sciences	0	0	0	24,175	+24,175
SBIR/STTR	0	11,608	11,608	12,757	+1,149
Total, Materials Sciences and Engineering	**346,633**	**362,749**	**362,749**	**386,578**	**+23,829**
Chemical Sciences, Geosciences, and Biosciences					
Fundamental Interactions Research	72,757	75,999	75,999	75,999	0
Chemical Transformations Research	93,531	93,531	93,531	93,531	0
Photochemistry and Biochemistry Research	69,556	69,556	69,556	69,556	0
Energy Frontier Research Centers (EFRCs)	42,680	42,000	42,000	42,000	0
Energy Innovation Hubs—Fuels from Sunlight	24,237	24,237	24,237	24,175	-62
General Plant Projects (GPP)	5,950	600	600	600	0
SBIR/STTR	0	10,093	10,093	10,417	+324
Total, Chemical Sciences, Geosciences, and Biosciences	**308,711**	**316,016**	**316,016**	**316,278**	**+262**
Scientific User Facilities					
Synchrotron Radiation Light Sources	396,170	432,000	432,000	484,166	+52,166
High-Flux Neutron Sources	246,448	245,900	245,900	248,490	+2,590

	FY 2013 Current	FY 2014 Enacted	FY 2014 Current	FY 2015 Request	FY 2015 vs. FY 2014 Enacted
Nanoscale Science Research Centers (NSRCs)	100,500	100,885	100,885	118,798	+17,913
Other Project Costs	24,400	37,400	37,400	9,300	-28,100
Major Items of Equipment	54,500	45,000	45,000	42,500	-2,500
Research	26,691	42,498	42,498	32,168	-10,330
SBIR/STTR	0	27,481	27,481	29,522	+2,041
Total, Scientific User Facilities	**848,709**	**931,164**	**931,164**	**964,944**	**+33,780**
Subtotal, Basic Energy Sciences	**1,504,053**	**1,609,929**	**1,609,929**	**1,667,800**	**+57,871**
Construction					
Linac Coherent Light Source-II (LCLS-II), SLAC	0	75,700	75,700	138,700	+63,000
National Synchrotron Light Source-II (NSLS-II), BNL	47,203	26,300	26,300	0	-26,300
Total, Construction	**47,203**	**102,000**	**102,000**	**138,700**	**+36,700**
Total, Basic Energy Sciences	**1,551,256**	**1,711,929**	**1,711,929**	**1,806,500**	**+94,571**

SBIR/STTR Funding:

- FY 2013 transferred: SBIR $39,756,000 and STTR $5,154,000 (transferred out of BES in FY 2013 Current column)
- FY 2014 projected: SBIR $43,035,000 and STTR $6,147,000
- FY 2015 Request: SBIR $46,309,000 and STTR $6,387,000

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Explanation of Major Changes ($K)

	FY 2015 vs. FY 2014 Enacted
Materials Sciences and Engineering: Core research activities will be supported at approximately the same level as FY 2014. The Batteries and Energy Storage Hub and Energy Frontier Research Centers will continue at the planned level. A new activity for computational materials sciences will be initiated that emphasizes integrated theoretical and experimental research, approaches to derive new knowledge from large experimental and theory/modeling data sets, and community software to accelerate discovery and advancement of functional materials for energy-use inspired applications.	+23,829
Chemical Sciences, Geosciences, and Biosciences: Core research activities will be supported at approximately the same level as FY 2014. The Energy Frontier Research Centers will continue at the planned level. The Fuels from Sunlight Hub receives the final year of funding for its five-year award term at the planned level in FY 2014. A decision for continued funding beyond the initial five year term, which ends in September 2015, will be made in FY 2015.	+262
Scientific User Facilities: BES will increase support for the operations of four light sources, five Nanoscale Science Research Centers (NSRCs), and two neutron sources at optimal levels. Funding will increase for early operations of the National Synchrotron Light Source-II (NSLS-II) that will transition from a construction project to operations in FY 2015. The National Synchrotron Light Source (NSLS) will cease operations and funds are provided to transition the facility to a safe storage condition in FY 2015. The BES operations at the Lujan Neutron Scattering Center will cease and funds are provided to transition the facility to a safe storage condition. The three electron beam microcharacterization centers will be merged administratively with their respective neighboring NSRCs in FY 2015. Funding for the APS Upgrade and NEXT MIE projects will continue per the project plans. Funding for Other Project Costs (OPC) for the LCLS-II construction project will decrease per the project plans.	+33,780
Construction: Construction of the NSLS-II will be ramped down as the project is completed in FY 2015, as scheduled. Construction of the LCLS-II will continue, as scheduled.	+36,700
Total, Basic Energy Sciences	**+94,571**

Basic and Applied R&D Coordination

As a fundamental research program within the Department of Energy, BES strives to build and maintain close connections with other DOE program offices. The Department facilitates coordination between DOE R&D programs through a variety of Departmental activities, including joint participation in research workshops, strategic planning activities, solicitation development, and program review meetings. For example, the DOE Hub Working Group meets regularly to coordinate programmatic oversight and promote commonality across the DOE Energy Innovation Hubs. BES also 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.

BES program managers regularly participate in intra-departmental meetings for information exchange and coordination on solicitations, program reviews, and project selections in the research areas of biofuels derived from biomass; solar energy utilization; 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 DOE technology offices and defense programs. DOE program managers have also established formal technical coordination working groups that meet on a regular basis to discuss R&D programs with wide applications for basic and applied programs including the Office of Environmental Management. Additionally, DOE technology office personnel participate in reviews of BES research, and BES personnel participate in reviews of research funded by the technology offices and ARPA-E. In FY 2015, Departmental leadership has identified crosscutting activities of particular emphasis for coordination between DOE programs. BES will collaborate with the Offices of Energy Efficiency and Renewable Energy, Fossil Energy, Electricity Delivery and Energy Reliability, and Nuclear Energy on a crosscut on subsurface engineering.

Co-funding and co-siting of research by BES and DOE technology programs at the same institutions 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 expertise and knowledge of research breakthroughs and program needs. The Department's national laboratory system plays a particularly important role in achieving integration of basic and applied research.

Program Accomplishments

Designing new materials. Understanding how to control the structure and composition of materials is foundational to the design of better materials. Major advances have recently been made across a wide spectrum of materials, such as:

- Using a combination of theory and experiment, extreme nano-structuring (e.g., fabricating very narrow wires or thin films perforated with many holes) was found to improve the performance of superconductors—materials which conduct electricity with no losses—in high magnetic fields. Nanostructured superconductors hold promise for practical use in the electricity grid and developing powerful electric motors.
- A new approach to self-assembly has provided 3-dimensional hierarchical architectures made-up of functionalized graphene (single layers of carbon atoms) with nanometer sized and larger diameter pores. The modified material exhibits enhanced electrochemical activity for possible use in high-capacity lithium-air batteries.
- Neutron scattering has uncovered the role of water in controlling the assembly of molecules, opening new avenues to control nanostructure in protein-based materials with important potential applications in bio-catalysis and energy conversion.

Ultrafast x-rays elucidate chemical transformations. The ultrashort x-ray pulses produced by the Linac Coherent Light Source (LCLS) at SLAC National Accelerator Laboratory are enabling unprecedented investigations into fundamental chemical processes for a wide range of important energy systems.

- By capturing short-time snapshots of a catalytic process, scientists proved the existence of transient precursor species on a catalytic surface, providing a missing link in the understanding of molecular-level chemical catalytic mechanisms and facilitating catalyst design for highly-efficient and selective chemical conversions.

- The high intensity of the x-ray pulses and their coherence has made possible imaging of individual aerosol particles in their airborne state, revealing structures of surprising diversity and complexity.
- Atomic positions and electronic structure were simultaneously analyzed in photo-activated Photosystem II, which is a key photosynthetic complex that converts light into chemical energy.

Scientific advances enable cleaner fossil energy. There continue to be scientific challenges to cleaner delivery of fossil energy. Among these are the design and discovery of new processes and materials for chemical separations, more reliable and effective carbon capture, and safe injection of carbon dioxide into geologic formations. Recent research results at the EFRCs have advanced the science in a number of areas, such as:

- New classes of novel molecular compounds have been discovered that can be functionalized to enable energy-efficient, lower-cost hydrocarbon separation with the potential to replace current energy-intensive gas separation processes.
- Computer simulations have screened thousands of possible materials and revealed promising options for the efficient separation of carbon dioxide from coal power plants and for methane capture from dilute and medium-concentration sources.
- Monitoring sub-surface carbon dioxide migration after geologic sequestration has been enabled by high-resolution seismic imaging and new computational algorithms.
- To further enhance understanding of how geological formations interact with stored carbon dioxide, experiments and computational modeling have been applied to derive a new fundamental understanding of how nanoscale features of rock surfaces control the growth and distribution of solid carbonates, the favored form of carbon sequestration in geologic formations.

Generating electricity from waste heat. Roughly 60% of the energy used in the world ends up as waste heat. Devices based on thermoelectric materials can convert waste heat to electricity. Research efforts at the EFRCs are addressing the scientific breakthroughs needed to control the flow of heat and electricity in these materials, advances that are critical to increasing the efficiency and decreasing the cost of thermoelectric devices.

- Experiments and theoretical models have demonstrated that the vibrations that carry heat across materials can travel in a wavelike fashion through a stack of thin films, suggesting new ways to engineer thermoelectric materials.
- Other experiments confirmed theoretical predictions that substituting specific atoms in materials reduces the thermal conductivity, providing an alternate approach to improve device efficiency.
- Use of earth abundant minerals in thermoelectric applications could significantly reduce manufacturing costs; theoretical modeling has made significant advances in this area, guiding the synthesis of new thermoelectric materials based on earth abundant minerals that perform comparably to existing thermoelectric materials.

New capabilities at light source facilities enable ground breaking science. From the powerful x-ray laser to an innovative device, researchers from various scientific communities employing instrumentation at synchrotron light sources to accomplish significant scientific discoveries.

- Researchers have demonstrated for the first time how to produce pairs of x-ray laser pulses in slightly different wavelengths with finely adjustable time intervals between them. Each of the paired x-ray laser pulses can be tuned to study a specific element in atomic detail, and they can be timed to hit a sample in very quick succession. This capability opens up a new realm of experiments at the Linac Coherent Light Source, potentially revealing how bonds between atoms form, break and rearrange, and how atoms absorb light on ultrafast time scales of less than 25 femtoseconds.
- A prototype superconducting undulator has successfully delivered first hard x-rays at the Advanced Photon Source. The new undulators can achieve twice the x-ray energy of existing devices, while still maintaining sufficient magnetic fields to provide high flux of hard x-rays. This breakthrough achievement has realized a long-standing objective of accelerator science to take advantage of the high current densities made possible by superconducting magnet technology to greatly enhance the performance of synchrotron light sources.

- The 2012 Nobel Prize in Chemistry was awarded for the breakthrough studies of G-protein-coupled receptors (GPCRs) enabled by advanced instruments at the Advanced Photon Source. GPCRs are a large set of proteins embedded in a cell's membrane that sense molecules outside the cell and activate a cascade of different cellular processes in response. They constitute key components of how cells interact with their environments and are the target of nearly half of today's pharmaceuticals.

BES user facilities assist industry to advance technologies and develop new drugs. Researchers from industry use the unique capabilities provided at the BES scientific user facilities to develop new technologies and new drugs that impact lives. BES researchers have collaborated with industry to:

- Combine a new low-temperature nanocrystalline diamond deposition technology and an efficient semiconductor doping process to produce highly n-type diamond films. The combination of this novel nanomaterial synthesis and understanding of the material structural and electronic properties are fundamental to realizing efficient very high power electronic devices. The research opens a commercially feasible approach to produce cheaper and better integrated circuits that could potentially transform energy, telecommunications, defense, and aviation electronics.
- Employ the protein crystallography techniques available at BES synchrotron light sources to understand how diseases function and to develop potential drugs for treatment. BES light source facilities have played a crucial role for those developments, such as a recently FDA-approved drug that treats type 2 diabetes in adults and a cancer drug, an angiogenesis inhibitor, that interferes with the growth of new blood vessels needed for solid cancer tumors to survive.
- Study the pore structure of oil and gas containing Barnett shale using small angle neutron scattering at the High Flux Isotope Reactor. The researchers analyzed the pore size distribution in different shale samples and the percentage of pores accessible to methane and water. The results helped shed light on why shales of similar compositions produced differing amounts of gas, and could inform the fracking process.

Description

Materials are critical to nearly every aspect of energy generation and end-use. Materials limitations are often the barrier to improved energy efficiencies, longer lifetimes of infrastructure and devices, or the introduction of new energy technologies. The *Materials Sciences and Engineering* subprogram supports research to provide the understanding of materials synthesis, behavior, and performance that will enable solutions to these wide-ranging challenges as well as opening new directions that are not foreseen based on existing knowledge. The research explores the origin of macroscopic material behaviors; their fundamental connections to atomic, molecular, and electronic structures; and their evolution as materials move from nanoscale building blocks to mesoscale systems. At the core of the subprogram is the quest to enable the predictive design and discovery of new materials with novel structures, functions, and properties. Such understanding and control are critical to science-guided design of highly efficient energy conversion processes, such as the conversion of sunlight to electricity, new electromagnetic pathways for enhanced light emission in solid-state lighting, and multi-functional nanoporous structures for optimum ionic and electronic transport in batteries and fuel cells.

To accomplish these goals, the portfolio includes three integrated research activities:

- **Scattering and Instrumentation Sciences**—Advancing new tools and techniques to characterize and correlate materials performance, structure, and dynamics on multiple time and length scales and in the environments in which materials are used.
- **Condensed Matter and Materials Physics**—Understanding the foundations of material functionality and behavior.
- **Materials Discovery, Design, and Synthesis**—Developing novel synthesis strategies to design and precisely assemble structures in order to control materials properties, enabling discovery of new materials with unprecedented functionalities.

The portfolio emphasizes understanding of how to direct and control energy flow in materials systems over multiple time and length scales, with increasing emphasis on the mesoscale. The research will enable prediction of materials behavior, transformations, and processes in challenging real-world systems—for example, for materials with many atomic constituents, complex structures, and a broad range of defects that are exposed to extreme environments. To maintain leadership in materials discovery, the research explores new frontiers and unpredicted, emergent materials behavior in materials systems, utilization of nanoscale control, and systems that are metastable or far from equilibrium. Finally, the research includes investigation of the interfaces between physical and biological sciences to explore bio-mimetic processes as new approaches to novel materials design. This subprogram is also the home of the DOE Experimental Program to Stimulate Competitive Research (EPSCoR) that supports research spanning the broad range of DOE's science and technology programs in states that have historically received relatively less Federal research funding in the university sector.

In addition to single-investigator and small-group research, the subprogram supports EFRCs and the Batteries and Energy Storage Energy Innovation Hub. These research modalities support multi-investigator, multidisciplinary research and focus on forefront energy technology challenges. The EFRCs support teams of investigators to perform basic research to accelerate transformative solutions for a wide range of energy technologies. The Batteries and Energy Storage Hub supports a large, tightly integrated team and research that spans basic and applied regimes with the goal of providing the scientific understanding that will enable the next generation of electrochemical energy storage for vehicles and the electrical grid. A new activity proposed for FY 2015 will support integrated, multidisciplinary teams of theorists and experimentalists that will focus on computational materials science to develop validated community codes for predictive design of functional materials. This activity will also support new approaches that enhance the use of the large data sets derived from advanced materials characterization of materials synthesis, processing, and properties assessments and the parallel data that are generated by large scale computational efforts on theory and modeling of materials phenomena.

Scattering and Instrumentation Sciences Research

Advanced characterization tools with very high precision in space and time are essential to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels. These capabilities provide the foundation for research central to DOE missions in energy, environment, and national security. Research in Scattering and Instrumentation Science supports innovative science, techniques, and instrumentation for scattering, spectroscopy, and imaging using electrons, neutrons, and x-rays. These tools provide precise information on the atomic structure and dynamics in materials. DOE's longstanding investments in world-leading electron, neutron, and synchrotron x-ray scattering facilities and the large associated user communities are a testament to the importance of this activity to the DOE mission. Revolutionary advances in these techniques will enable transformational research on advanced materials to address energy challenges.

The unique interactions of electrons, neutrons and x-rays with matter enable a range of complementary tools with different sensitivities and resolution for the characterization of materials at length- and time-scales spanning several orders of magnitude. Recent advances in investigations of dynamic phenomena in real-time and relevant conditions provide a window into material functions under the conditions in which the materials are used. New instrumentation in the ultrafast regime will be used to investigate dynamics at very fast timescales related to electronic, catalytic, magnetic, and other transport processes. A distinct aspect of this activity is the development of innovative instrumentation concepts and techniques for neutron scattering and imaging needed to correlate the microscopic and macroscopic properties of energy materials. Characterization for mesoscale phenomena are growing aspects of this research.

Condensed Matter and Materials Physics Research

Understanding the foundations of how to control and change the properties of materials is critical to improving their functionality on every level and is essential to fulfilling DOE's energy mission. The Condensed Matter and Materials Physics activity supports experimental and theoretical research to advance our current understanding of phenomena in condensed matter—solids with structures that vary in size from the nanoscale to the mesoscale, the materials that make-up the infrastructure for energy technologies, including electronic, magnetic, optical, thermal, and structural materials.

A central focus is research to characterize and understand materials whose properties are derived from the strong interactions of the electrons in their structure, such as superconductors and magnetic materials. An emphasis is placed on investigating low-dimensional systems, including nanostructures, and studies of the electronic properties of materials under extreme conditions such as ultra-low temperatures and extremely high magnetic fields. The research is relevant to energy technologies and advances the fundamental understanding of the elementary energy conversion steps related to photovoltaics and solid state lighting, the energetics of hydrogen storage, and electron spin-phenomena and basic semiconductor physics relevant to next generation information technologies and electronics. Fundamental studies of the quantum mechanical behavior of electrons in materials will lead to an improved understanding of electrical and thermal conduction in a wide range of material systems. There is a critical need to couple theories that describe properties at the atomic scale to properties at the macroscale where the influence of size, shape, and composition is not adequately understood.

The activity also emphasizes understanding how materials respond to their environments, including temperature, electromagnetic fields, radiation, and chemical environments. This includes the defects in materials and their effects on materials' electronic properties, strength, structure, deformation, and failure over a wide range of length and time scales that will enable the design of materials with superior properties and resistance to change under the influence of radiation.

Materials Discovery, Design, and Synthesis Research

The discovery and development of new materials has long been recognized as the engine that drives science frontiers and technology innovations. Predictive discovery of new forms of matter with tailored properties is still a significant challenge for materials sciences. A strong, vibrant research enterprise in the discovery of new materials is critical to world leadership—scientifically, technologically and economically. One of the goals of this activity is to grow and maintain U.S.

leadership in materials discovery by investing in advanced synthesis capabilities and by coupling these with state-of-the-art user facilities and advanced computational capabilities at DOE national laboratories.

A key part of this portfolio is bio-mimetic and bio-inspired materials research—translating biological processes into impactful approaches to the design and synthesis of materials with the remarkable properties found in nature, e.g., self-repair and adaptability to the changing environment. Synthesis science and materials chemistry research underpin many energy-related technological areas such as batteries and fuel cells, catalysis, solar energy conversion and storage, friction and lubrication, and membranes for advanced separations, efficient ion transport and highly selective gas separation and storage.

Major research directions include the controlled synthesis of nanoscale materials and their assembly into functional materials with desired properties; porous materials with tailored reactivities and porosities; mimicking the energy-efficient synthesis approaches of biology to generate new, advanced materials for use under harsher, non-biological conditions; bio-inspired materials that assemble autonomously and, in response to external stimuli, dynamically assemble and disassemble; and adaptive and resilient materials that also possess self-repairing capabilities. Synthesis science supports fundamental research on the development of new methods and techniques to synthesize materials with targeted structure and properties. An important element of this activity is the development of real-time monitoring tools, diagnostic techniques, and instrumentation that can provide information on the progression of structure and properties as a material is formed, in order to understand the underlying physical mechanisms and to gain atomic level control of material synthesis and processing.

Experimental Program to Stimulate Competitive Research (EPSCoR)

DOE's Experimental Program to Stimulate Competitive Research (EPSCoR) is a Federal-State partnership program designed to enhance the capabilities and research infrastructure of designated states and territories to conduct sustainable and nationally competitive research. This activity supports basic research spanning the broad range of science and technology related to DOE mission areas in states and territories that have historically received relatively less Federal research funding than other states. EPSCoR helps these states develop their capabilities so that they can successfully compete for research funding. The EPSCoR program supports 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, electricity delivery and reliability, nuclear energy, and energy efficiency and renewable energy.

EPSCoR promotes strong research collaboration between scientists/engineers in the designated states/territories and the world-class national laboratories, leveraging national user facilities and taking advantage of opportunities for intellectual collaboration across the DOE system. DOE EPSCoR supports Implementation Grants (large grants that promote development of infrastructure and research teams) and State-Laboratory partnership grants (individual university-based principal investigators teaming with national laboratories). EPSCoR is science-driven and supports the most meritorious proposals based on peer review and programmatic priorities.

Energy Frontier Research Centers (EFRCs)

The EFRCs, initiated as five-year awards in FY 2009 and undergoing a full recompetition in FY 2014, are a unique and important research modality, bringing together the skills and talents of teams of investigators to perform energy-relevant, basic research with a scope and complexity beyond that possible in standard single-investigator or small-group awards. These multi-investigator, multi-disciplinary centers foster, encourage, and accelerate basic research to provide the basis for transformative energy technologies. The EFRCs are funded on a continuing basis through annual appropriations through this subprogram and the Chemical Sciences, Geosciences, and Biosciences subprogram. The EFRCs supported in this subprogram 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 and fuels and that enhance the conversion of electricity to light; the development of the understanding of materials and processes required to enable improved electrical energy storage and to increase materials resistance to corrosion, decay, or failure in extreme conditions of temperature, pressure, radiation, or chemical exposures; and the exploration of emergent phenomena, such as superconductivity, that can optimize energy flow and boost the efficiency of energy transmission. At the end of FY 2013, after four years of research activity, the 46 EFRCs had produced an impressive breadth of accomplishments, including over 4,000 peer-reviewed journal papers, over 200 patent applications and over 90 additional patent/invention disclosures.

BES's active management of the EFRCs continues to be an important feature of the program. A variety of methods are used to regularly assess the progress of the EFRCs, including annual progress reports, monthly phone calls with the EFRC Directors, periodic Directors' meetings, and on-site visits by program managers. BES also conducts in-person reviews by outside experts. Each EFRC undergoes a review of its management structure and approach in the first year of the award and a midterm assessment of scientific program and progress compared to its 5-year scientific goals. To facilitate communication of results to other EFRCs and interactions with DOE technology programs, meetings of the EFRC principal investigators are held on an approximately biennial frequency.

An open recompetition of the EFRC program is taking place in FY 2014. New and renewed EFRCs will be selected based on peer review by external experts. All of the EFRCs will continue to emphasize both grand challenge science and energy use-inspired research. Compared to the original awards, these EFRCs will include topics in mesoscale science and an enhanced focus on predictive materials and chemical sciences. Another change is that these will be 3-year initial awards with the extension for the remaining 2-years of the 5-year period dependent on the outcome of the mid-term peer review. This change will allow optimization of the portfolio at the midterm assessment, bolstering the strongest performers and eliminating the weakest performing activities as appropriate. In FY 2015, the EFRCs awarded in FY 2014 will undergo a peer review to ensure a strong start-up of their research programs and to provide a critical assessment of their management structures.

Energy Innovation Hubs (Batteries and Energy Storage)

Advanced energy storage solutions have become increasingly critical to the Nation with the expanded deployment of renewable energy sources coupled with growth in the numbers of hybrid and electric vehicles. For the electric grid, new approaches to electrochemical energy storage can provide enhanced grid stability and enable intermittent renewable energy sources to meet continuous electricity demand. For vehicles, new batteries with improved lifetimes, safety, and storage capacity are needed to expand the range of electric vehicles from a single charge while simultaneously decreasing the volume, manufacturing cost and weight. Today's electrical energy storage approaches suffer from limited energy and power capacities, lower-than-desired rates of charge and discharge, life-cycle limitations, low abuse tolerance, high cost, and decreased performance at high or low temperatures.

The Batteries and Energy Storage Hub, established in December 2012, focuses on understanding the fundamental performance limitations for electrochemical energy storage to launch the next generation, beyond lithium-ion energy storage technologies relevant to both the electric grid and transportation. The Hub, the Joint Center for Energy Storage Research (JCESR), is led by Argonne National Laboratory joined by four other national laboratories, five universities, and four industrial partners. JCESR's core task is basic research—using a new generation of nanoscience tools that enable observation, characterization, and control of matter down to the atomic and molecular scales to understand materials and chemical processes that are at the core of battery performance. The participation of industrial partners will facilitate efforts to ensure that the outcome of basic research leads toward practical solutions that are competitive in the marketplace.

JCESR focuses on systems beyond lithium-ion and discovery of new energy storage chemistries through the development of an atomic-level understanding of reaction pathways and development of universal design rules for electrolyte function. The overarching goals driving the scientific and engineering research towards next-generation energy storage technologies are summarized by JCESR as 5/5/5—five times the energy density of current systems at one-fifth the cost within five years, the award period for the Hub. In addition, JCESR will deliver two additional legacies to the broader energy storage community: creation of a library of fundamental scientific knowledge of the phenomena and materials of energy storage at the atomic and molecular level and demonstration of a new paradigm for battery R&D—integrating discovery science, battery design and computation, and research prototyping in a single highly interactive organization. Success in achieving these legacies will be measured by the rate, quality, and impact of JCESR's scientific publications, patents, and interactions across its discovery science, battery design and computation, and research prototyping functions. Progress against milestones is evaluated by quarterly/annual reports and annual performance reviews by external panels of science and management experts to verify and validate performance.

Computational Materials Sciences

Recent major strides in materials synthesis, processing, and characterization, combined with concurrent advances in computational science—enabled by improvements in high performance computing capabilities—have opened an unprecedented opportunity to design new materials with specific properties. The opportunity is to leap beyond simple extensions of current theory and models of materials towards a paradigm shift in which specialized computational codes and software enable the ability to design, discover, and develop new materials, and in turn, create new advanced, innovative technologies. Given the importance of materials to virtually all technologies, computational materials sciences is a critical area in which the United States needs to be competitive.

If successful, this paradigm shift would significantly accelerate the design of revolutionary materials to meet the Nation's energy goals and enhance economic competitiveness. Development of fundamentally new design principles could enable stand-alone research codes and software packages to address multiple length and time scales for prediction of the total functionality of materials over a lifetime of use. Recent scientific workshops and National Research Council studies have identified enticing scientific challenges that would advance these goals.[a] Examples include dynamics and strongly correlated matter, conversion of solar energy to electricity, design of new catalysts for a wide range of industrial uses, and transport in materials for improved electronics. Success will require extensive research and development with the goal of creating experimentally validated, robust community codes that will enable functional materials innovation.

Research and development to create the computational codes will require a fully integrated team approach, combining the skills of experts in materials theory, modeling, computation, synthesis, characterization, and processing/fabrication. The range of the research will include development of new ab initio theory, mining the data from both experimental and theoretical databases, performing advanced in situ/in operando characterization to generate the specific parameters needed for computational models, and well controlled synthesis to confirm the predictions of the codes. Many of the underlying phenomena require understanding the material dynamics at ultrafast time scales and with near atomic resolution—requiring effective use of the unique world leading tools and instruments at DOE's user facilities, from ultrafast free electron lasers to aberration corrected electron microscopes to the best tools for atomically controlled synthesis.

To facilitate U.S. leadership in this competitive field, FY 2015 funding is requested to support up to four large teams of scientists and engineers who would perform the basic research and develop and deliver codes and associated experimental/computational data for the design of functional materials. Each team would focus on a different area of functional materials; BES-led coordination among the teams would further leverage activities and accelerate key foundational research. A Funding Opportunity Announcement would solicit proposals from the materials research community, with the best proposals selected by peer review. Awards would be for five years, with the first year funded with FY 2015 funding. An ideal end product would be open source, robust, validated, user friendly software that captures the essential physics and chemistry of relevant systems and can be used by the broader research community and by industry to dramatically accelerate the design of new functional materials. Following the effective management approach employed with other large team research activities, BES will actively manage the project through annual peer reviews to assess progress towards planned scientific goals.

[a] U.S. DOE. *Computational Materials Science and Chemistry for Innovation*. U.S. Department of Energy Office of Science, 2010. National Research Council. Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security. Washington, DC: The National Academies Press, 2008.

Activities and Explanation of Changes

FY 2014 Enacted	FY 2015 Request	Explanation of Changes FY 2015 vs. FY 2014 Enacted
Scattering and Instrumentation Sciences Research		
Research continues to emphasize the opportunities afforded by x-ray, neutron and electron scattering, spectroscopy, and imaging for the development of new functional materials for energy production, storage, and distribution. Scattering science enables unique insights into the structure and dynamics of new energy materials over relevant time and length scales. Research advances the development and utilization of new capabilities with increasing physical, chemical, structural, and temporal precision for materials research. Research on soft and hybrid materials is emphasized. New research advances the use of ultrafast techniques to tackle research challenges in materials sciences.	Time domain, energy spectroscopy, and *in situ* instrumentation continues to improve, allowing advanced investigations of excitation and transport with high spatial resolution across relevant length scales for energy systems. Integration of multiple sources and detection schemes will be emphasized to provide more complete assessment of spatial structures and excitation levels with high time resolution. Quantitative pictures of complex materials as they evolve in time under realistic environmental boundary conditions will validate theory and increase phenomenological understanding. Spatial resolution will span atoms to microstructure, including the mesoscale. Time scales to be investigated involve electronic motion in the ultra-fast regime, cooperative modes at atomic vibration and diffusion time scales, and degradation time scales across mesoscale structures.	Research support is flat compared to FY 2014. Areas of increased emphasis include ultrafast materials science, in situ, under operational conditions, time-resolved imaging, and energy excitation spectroscopy with high spatial resolution; all directed towards understanding scientific phenomena on real systems at realistic operating conditions. Mature use of recently established techniques (such as high pressure cell studies and metallurgical orientational imaging) will be de-emphasized as these are now being implemented more routinely by researchers investigating particular materials systems.

FY 2014 Enacted	FY 2015 Request	Explanation of Changes FY 2015 vs. FY 2014 Enacted
Condensed Matter and Materials Physics Research		
Research continues to emphasize experimental and theoretical research on materials that exhibit correlation effects, including new phenomena observed in topological surface states and the development of new theoretical tools and validated software for materials discovery that is relevant to energy technologies. Research focuses on advancing fundamental understanding of defects in materials, which is needed to extend the lifetime and enhance the performance of materials used in energy generation and energy end-use technologies. This activity supports research on large, ultra-cold atom clusters that can exhibit both bosonic or ferminoic behavior to provide new insights into the evolution of condensed matter behavior. There is continued support for research on understanding structure-property relationships in materials by studying the influence of reduced dimensionality and defects on the physical, optical, and electrical properties of materials; and controlling material functionality in response to external stimuli such as temperature, pressure, magnetic and electric fields, and radiation.	Research will continue to support experimental and theoretical materials research emphasizing correlation effects, including phenomena observed in topological surface states. The program will emphasize the development of understanding of matter at atomistic length scales expanding to include properties at the mesoscale. This includes research on cold atom clusters to determine if these systems can provide new insights into the evolution of condensed matter behavior from atomic constituents. The program supports research on phenomena that occur as a consequence of interfaces and reduced dimensionality. Research will continue to include assessments of the phenomena related to the structural, optical, and electrical properties of materials; and the control of material functionality in response to external stimuli including temperature, pressure, magnetic and electric fields, and radiation. The program will continue to grow research on new theoretical tools and validated software for materials discovery. The research will continue to advance fundamental understanding of defects to extend the lifetime and enhance performance of materials in energy generation and energy end-use applications.	Research support is flat compared to FY 2014. The FY 2015 program enhances research on predictive materials design and experimental validation. The program will also expand research focused on our understanding of matter at atomistic length scales expanding to include properties at the mesoscale. Research on granular materials and conventional superconductivity will be de-emphasized.

FY 2014 Enacted	FY 2015 Request	Explanation of Changes FY 2015 vs. FY 2014 Enacted
Materials Discovery, Design, and Synthesis Research		
Research continues on the development of guiding principles for the predictive design and synthesis of materials across multiple length scales—from atomic and molecular to nanoscale to mesoscale and ultimately to bulk. Predictive design of materials synthesis is coupled to experimental research on biology-inspired, physical, and chemical synthesis and processing techniques. This is made possible by effective integration of theory and experiment, modeling of synthetic pathways and experimental designs. Synthesis pathways may be precisely controlled by the use of in situ diagnostic tools and will pave the way for atom- and energy-efficient syntheses of new forms of matter with tailored properties. Research on understanding of carbon capture takes advantage of novel chemistries and approaches for gas storage and release, including innovative biomolecular materials research.	Research will continue to focus on the predictive design and synthesis of materials across multiple length scales, with a particular emphasis on the mesoscale. This will be enabled by more effective coupling of computational tools to experimental research on biology-inspired, physical, and chemical synthesis and processing techniques. Synthesis pathways may be better understood and precisely controlled by use of in situ diagnostic tools and characterization techniques, developed in the laboratory and at BES user facilities. This will create viable approaches for atom- and energy-efficient syntheses of new forms of matter with tailored properties. A key challenge will be to realize the complexity and functionality of biological systems, but with the use of inorganic earth-abundant materials. Research on novel materials for gas separations and storage will continue to take advantage of novel chemistries and concepts, including those inspired by biology.	Research support is flat compared to FY 2014. Research on developing synthesis methods for nanomaterials, e.g., nanoparticles, nanorods, etc. will be deemphasized in view of the recent progress on these topics. Research related to mesoscale phenomena and the building of mesoscale structures from nanoscale building blocks will be enhanced.
Experimental Program to Stimulate Competitive Research (EPSCoR)		
Efforts continue to span science in support of the DOE mission, with continued emphasis on science that underpins DOE energy technology programs. Meritorious Office of Science Early Career Research Program proposals from EPSCoR jurisdictions will be considered for support on a case-by-case basis. Funding for implementation grants is enhanced to minimize mortgages.	Research strengthens capabilities to advance DOE mission needs across energy science and technology in the EPSCoR states. Implementation grant and investment in early career research staff from EPSCoR states will be sustained.	Research support decreases compared to FY 2014. The additional funding provided in FY 2014 was used to support implementation grants with funding profiles that minimized outyear mortgages.

FY 2014 Enacted	FY 2015 Request	Explanation of Changes FY 2015 vs. FY 2014 Enacted
Energy Frontier Research Centers (EFRCs)		
A single Funding Opportunity Announcement (FOA) was issued for both renewal and new EFRCs for five-year awards beginning in FY 2014. The EFRC FOA encouraged the formation of effective teams to address the broad range of fundamental science needed to power transformative energy technologies, including newly identified opportunities in the computational design of materials and chemical processes and mesoscale science. All current EFRCs, including those initially funded through ARRA, had the opportunity to compete for a second five-year performance period. All awards, both new and renewal, will be based on rigorous peer review of the research proposed for the five year award term. Applicants requesting renewal funding will also be assessed on progress during the first five-year award.	The EFRCs that will be started in FY 2014 will perform the first year of research of the award period as outlined in their proposals. This multidisciplinary research will continue to provide accelerated progress in fundamental, energy-use inspired research. The research in these new EFRCs includes investigations of mesoscale science and utilization of computational research to predictably design new materials and processes. BES will hold a peer review to assess management and early operations.	FY 2015 support for EFRCs will continue at the FY 2014 level.
Energy Innovation Hubs—Batteries and Energy Storage		
Hub research on electrochemical energy storage continues to follow the plans established in the proposal as revised in the initial months of operation in consultation with DOE. Joint Center for Energy Storage Research (JCESR) operations and management processes are informed by the management review held in October 2013. A full peer review of the technical progress of the Hub research is scheduled for July 2014.	Research will continue to follow the established project plan for thrusts on multivalent intercalation, chemical transformations, and non-aqueous redox flow, as well as cross-cutting research on materials characterization, theory, and modeling. Systems analysis and translation activities will include techno-economic modeling, cell design, and preliminary prototype development. Research will include a focus on the electrolyte genome, demonstrating the utility of this computational framework for designing new electrolytes using structure-chemical trends extracted from >10,000 first-principles calculated molecular motifs, modifications and mutations.	The funding is approximately flat compared to FY 2014, following the planned funding profile.

FY 2014 Enacted	FY 2015 Request	Explanation of Changes FY 2015 vs. FY 2014 Enacted
Computational Materials Science		
	Coupling today's computational capabilities with world leading experimental instrumentation, Computational Materials Science will enhance U.S. leadership in the development of experimentally validated, robust computational codes that will enable materials discovery and innovation to meet the Nation's energy goals and enhance economic competitiveness. Funding will support up to four large teams of experts in materials theory, modeling, computation, synthesis, characterization, and processing/fabrication to perform the basic research required to develop and deliver research-oriented software and associated databases for predictive design of functional materials. In FY 2015, a competitive, peer review process will select the best research proposals, with each of the selected proposal teams focused on a different type of functional material. FY 2015 funding will support the first year of 5-year awards.	This is a new research activity for FY 2015. Areas of research opportunity have been identified by BES and other agency workshops and National Research Council studies. Potential research areas relevant to energy include dynamics and strongly correlated matter (magnets, superconductors), conversion of solar energy to electricity, transport in materials for improved electronics, and design of new catalysts. Unique to this new activity are the breadth of the theory-computation-experimental teams and the specific goal of delivering software open source packages and associated databases to address multiple length and time scales for discovery and prediction of the functionality of materials for energy applications.

Description

The transformation of energy between types (optical, electrical, chemical, heat, etc.) and the rearrangement of matter at the atomic, molecular, and nano-scales are critically important in every energy technology. The *Chemical Sciences, Geosciences, and Biosciences* subprogram supports research that explores fundamental aspects of chemical reactivity and energy transduction in order to develop a broad spectrum of new chemical processes, such as catalysis, that can contribute significantly to the advancement of new energy technologies. Research addresses the challenge of understanding physical and chemical phenomena over a tremendous range of spatial and temporal scales, from molecular through nanoscale and on to mesoscale, and at multiple levels of complexity, including the transition from quantum to classical behavior.

At the heart of this research lies the quest to understand and control chemical processes and the transformation of energy at the molecular scale in systems spanning simple atoms and molecules, active catalysts, and larger biochemical or geochemical systems. At the most fundamental level, the development and understanding of the quantum mechanical behavior of electrons, atoms, and molecules is rapidly evolving into the ability to control and direct such behavior to achieve desired results in meso- and macro-scale energy conversion systems.

This subprogram seeks to extend this new era of control science to include the capability to tailor chemical transformations with atomic and molecular precision. Here, the challenge is to achieve fully predictive assembly and manipulation of larger, more complex chemical, geochemical, and biochemical systems at the same level of detail now known for simple molecular systems.

To address these challenges, the portfolio includes coordinated research activities in three areas:

- **Fundamental Interactions**—Structural and dynamical studies of atoms, molecules, and nanostructures with the aim of providing a complete understanding of atomic and molecular interactions in the gas phase, condensed phase, and at interfaces.
- **Chemical Transformations**—Design, synthesis, characterization, and optimization of chemical processes that underpin advanced energy technologies, including catalytic production of fuels, nuclear energy, and geological sequestration of carbon dioxide.
- **Photochemistry and Biochemistry**—Research on the molecular mechanisms involved in the capture of light energy and its conversion into chemical and electrical energy through biological and chemical pathways.

The portfolio of this subprogram includes several unique efforts that enable these overall research themes. Novel sources of photons, electrons, and ions are developed to probe and control atomic, molecular, nanoscale, and mesoscale matter, particularly ultrafast optical and x-ray techniques to study and direct molecular, dynamics, and chemical reactions. This subprogram supports the nation's largest Federal effort in catalysis science for the design of new catalytic methods and materials for the clean and efficient production of fuels and chemicals. It also contains a unique effort in the fundamental chemistry of the heavy elements, with complementary research on chemical separations and analysis. Research in geosciences emphasizes analytical and physical geochemistry, rock-fluid interactions, and flow/transport phenomena that are critical to a scientific understanding of carbon sequestration. 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 on artificial systems includes organic and inorganic photochemistry, photo-induced electron and energy transfer, photoelectrochemistry, and molecular assemblies for artificial photosynthesis.

In addition to single-investigator and small-group research, the subprogram supports EFRCs and the Fuels from Sunlight Energy Innovation Hub. These research modalities support multi-investigator, multidisciplinary research and focus on forefront energy technology challenges. The Hub supports a large, tightly integrated team and research that spans basic and applied regimes with the goal of providing the scientific understanding that will enable the next generation of technologies for the direct conversion of sunlight to chemical fuels.

Fundamental Interactions Research

This activity builds the fundamental science basis essential for technological advances in a diverse range of energy processes. Research encompasses structural and dynamical studies of atoms, molecules, and nanostructures, and the description of their interactions in full quantum detail. The ultimate objective, often gained through studies of model systems, is a complete understanding of reactive chemistry in the gas phase, condensed phase, and at interfaces. In complement, this activity supports development of novel experimental and theoretical tools. New sources of photons, electrons, and ions are used to probe and control atomic, molecular, nanoscale, and mesoscale matter and processes on ultrafast time scales. New algorithms for computational chemistry are developed and applied in close coordination with experiment. Areas of emphasis are use-inspired, with relevance, for example, to combustion and catalysis, but the knowledge and techniques produced by this activity form a science base to underpin numerous aspects of the DOE mission.

The principal research thrusts are in atomic, molecular, and optical (AMO) sciences and chemical physics. AMO research emphasizes the interactions of atoms, molecules, and nanostructures with photons, particularly those from BES light sources, to characterize and control their behavior. AMO research examines energy transfer within isolated molecules that provides the foundation for understanding the making and breaking of chemical bonds. Chemical physics research builds from the AMO research foundation by examining reactive chemistry of molecules that are not isolated, but whose chemistry is profoundly affected by the environment. It explores the transition from molecular-scale chemistry to collective phenomena in complex systems, such as the effects of solvation or interfaces on chemical structure and reactivity. This transition is often accompanied by a parallel transition from quantum mechanical behavior to classical or continuum behavior. Understanding such collective behavior is critical in a wide range of energy and environmental applications, from solar energy conversion to improved methods for handling radiolytic effects in context of advanced nuclear fuel or waste remediation. Gas-phase chemical physics emphasizes the incredibly rich chemistry of combustion—burning diesel fuel involves thousands of chemical reactions and hundreds of distinct species. Combustion simulation and diagnostic studies address the subtle interplay between combustion chemistry and the turbulent flow that characterizes all real combustion devices. This activity includes support for the Combustion Research Facility, a multi-investigator research laboratory at the Sandia National Laboratories campus in Livermore, California, for the study of combustion science.

Chemical Transformations Research

Chemical Transformation Research emphasizes the design, synthesis, characterization, and optimization of chemical processes that underpin advanced energy technologies including the catalytic production of fuels, nuclear energy, and geological sequestration of carbon dioxide. A tremendous breadth of novel chemistry is covered: inorganic, organic, and hybrid molecular complexes; nanostructured surfaces; electrochemistry; nanoscale membranes; bio-inspired chemistry; and analytical and physical geochemistry. This activity develops unique tools for chemical analysis, using laser-based and ionization techniques for molecular detection, with an emphasis on imaging chemically distinct species.

This activity has a leadership role in the application of basic science to unravel the principles that define how catalysts work—how they accelerate and direct chemistry. Such knowledge enables the rational synthesis of novel catalysts, designed at the nanoscale but operating at the mesoscale, which will lead to increased energy efficiency and chemical selectivity. Because so many processes for the production of fuels and chemicals rely on catalysts, improving catalytic efficiency and selectivity has enormous economic and energy consequences. Advanced gas separation schemes for the removal of carbon dioxide from post-combustion streams are explored—these are essential to making carbon capture an economic reality. Fundamental studies of the structure and reactivity of actinide-containing molecules provides the basis for their potential use in advanced nuclear energy systems. Geosciences research emphasizes a greater understanding of the consequences of deliberate storage, or accidental discharges, of energy related products (carbon dioxide or waste effluents), which require ever more refined knowledge of how such species react and move in the subsurface environment.

Photochemistry and Biochemistry Research

This activity supports research on the molecular mechanisms that capture light energy and convert it into electrical and chemical energy in both natural and man-made systems. The work is of critical importance for the effective use of our most abundant and durable energy source—the sun. More energy from the sun strikes the earth in one hour than is used by its entire human population in a year.

Natural photosynthesis is studied to provide roadmaps for the creation of robust artificial and bio-hybrid systems that exhibit the biological traits of self-assembly, regulation, and self-repair and that span from the atomic scale through the mesoscale. Physical science tools are extensively utilized to elucidate the molecular and chemical mechanisms of biological energy transduction, including processes beyond primary photosynthesis such as carbon dioxide reduction and subsequent deposition of the reduced carbon into energy-dense carbohydrates and lipids. Complementary research on artificial systems encompasses organic and inorganic photochemistry, light-driven energy and electron transfer processes, as well as photo-electrochemical mechanisms and molecular assemblies for artificial photosynthetic fuel production.

Energy Frontier Research Centers

The EFRCs, initiated as five-year awards in FY 2009 and undergoing a full recompetition in FY 2014, are a unique and important research modality, bringing together the skills and talents of teams of investigators to perform energy-relevant, basic research with a scope and complexity beyond that possible in standard single-investigator or small-group awards. These multi-investigator, multi-disciplinary centers foster, encourage, and accelerate basic research to provide the basis for transformative energy technologies. The EFRCs are funded on a continuing basis through annual appropriations through this subprogram and the Materials Sciences and Engineering subprogram. The EFRCs supported in this subprogram are focused on the design, discovery, control, and characterization of the 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. At the end of FY 2013, after four years of research activity, the 46 EFRCs had produced an impressive breadth of accomplishments, including over 4,000 peer-reviewed journal papers, over 200 patent applications and over 90 additional patent/invention disclosures.

BES's active management of the EFRCs continues to be an important feature of the program. A variety of methods are used to regularly assess the progress of the EFRCs, including annual progress reports, monthly phone calls with the EFRC Directors, periodic Directors' meetings, and on-site visits by program managers. BES also conducts in-person reviews by outside experts. Each EFRC undergoes a review of its management structure and approach in the first year of the award and a midterm assessment of scientific program and progress compared to its 5-year scientific goals. To facilitate communication of results to other EFRCs and interactions with DOE technology programs, meetings of the EFRC principal investigators are held on an approximately biennial frequency.

An open recompetition of the EFRC program is taking place in FY 2014. Renewing and new EFRCs will be selected based on peer review by external experts. All of the EFRCs will continue to emphasize both grand challenge science and energy use-inspired research. Compared to the original awards, these EFRCs will include topics in mesoscale science and an enhanced focus on predictive materials and chemical sciences. Another change is that these will be 3-year initial awards with the extension for the remaining 2-years of the 5-year period dependent on the outcome of the mid-term peer review. This change will allow optimization of the portfolio at the midterm assessment, bolstering the strongest performers and eliminating the weakest performing activities as appropriate. In FY 2015, the EFRCs awarded in FY 2014 will undergo a peer review to ensure a strong start-up of their research programs and to provide a critical assessment of their management structures.

Energy Innovation Hubs—Fuels from Sunlight

Solar energy is a significant yet largely untapped clean energy resource. More energy from the sun strikes the earth in one hour than is consumed by all humans on the planet in a year. Through the process of photosynthesis, plants can effectively convert energy from the sun into energy-rich chemical fuels using the abundant feedstocks of water and carbon dioxide. If a human-made artificial photosynthesis system can be developed that can generate usable fuels directly from sunlight, carbon dioxide, and water, the potential energy benefits for the Nation would be substantial, reducing dependence on fossil fuels through use of fuels generated directly by sunlight. Due to the significant scientific and engineering challenges associated with developing such a system, however, there are no commercially-available fuels generated via artificial photosynthesis. For this reason, the Basic Energy Sciences Advisory Committee report, New Science for Secure and Sustainable Energy Future,[a] listed the production of fuels directly from sunlight as one of three strategic goals for which transformational science breakthroughs are most urgently needed.

Established in September 2010, the Fuels from Sunlight Hub, the Joint Center for Artificial Photosynthesis (JCAP), is a multi-disciplinary, multi-investigator, multi-institutional effort to create critical transformative advances in the development of artificial photosynthetic systems for converting sunlight, water, and carbon dioxide into a range of commercially useful fuels. The Hub is targeted towards understanding and designing catalytic complexes or solids that generate chemical fuel from carbon dioxide and/or water; integrating all essential elements, from light capture to fuel formation components, into an effective solar fuel generation system; and providing a pragmatic evaluation of the solar fuel system under development. JCAP is led by the California Institute of Technology (Caltech) in primary partnership with Lawrence Berkeley National Laboratory (LBNL). Other partners include the SLAC National Accelerator Laboratory and several University of California institutions. JCAP is composed of internationally renowned scientists and engineers who seek to integrate decades of research community efforts and address critical research and development gaps; its visionary goal is the construction of an artificial photosynthetic system for robustly producing fuel from the sun ten times more efficiently than current crops.

Research in JCAP ranges from fundamental discovery of new materials to science-based design and testing of fully functional prototypes. JCAP has eight major parallel research and development projects: light capture and conversion; heterogeneous catalysis; molecular catalysis; high throughput experimentation; catalyst and photochemical benchmarking; molecular-nanoscale interfaces; membrane and mesoscale assembly; and prototyping. The projects' efforts are synergistically split between JCAP-South on the campus of CalTech and JCAP-North located near LBNL, with the exception of the benchmarking and high-throughput experimentation projects that are consolidated at JCAP-South. JCAP also makes use of state-of-the-art facilities at LBNL and SLAC as part of their efforts to examine, understand, and manipulate matter at the nanoscale. Despite the different geographic locations, JCAP is designed to operate as a single scientific entity. Its current efforts consist of discovery research to identify robust, Earth-abundant light absorbers, catalysts, linkers, and membranes that are required components of a complete system and scale-up science for design and development of prototypes. By studying the science of scale-up and by benchmarking both components (catalysts) and systems (device prototypes), JCAP seeks to move bench-top discovery to proof-of-concept prototyping and thus accelerate the transition from laboratory discovery to industrial use.

The Fuels from Sunlight Hub receives the final year of funding of its initial five-year award term at the planned level in FY 2014. A decision for continued funding beyond the initial term, which ends in September 2015, will be made in FY 2015.

General Plant Projects (GPP)

GPP funding is provided for minor new construction, for other capital alterations and additions, and for improvements to land, buildings, and utility systems at the Ames Laboratory. Funding of this type is essential for maintaining the productivity and usefulness of Department-owned facilities and for meeting requirements for safe and reliable facilities operation. The total estimated cost of each GPP project will not exceed $10,000,000.

[a] U.S. DOE Basic Energy Sciences Advisory Committee. *New Science for Secure and Sustainable Energy Future*. U.S. Department of Energy Office of Science, 2008.

Activities and Explanation of Changes

FY 2014 Enacted	FY 2015 Request	Explanation of Changes FY 2015 vs. FY 2014 Enacted
Fundamental Interactions Research		
AMO sciences research continues to emphasize the development and application of forefront ultrafast x-ray and optical probes of matter, utilizing the Linac Coherent Light Source and BES synchrotron light sources, and new theoretical methods for the interpretation of ultrafast measurements. Increasing emphasis is being placed on novel x-ray probes of matter, including non-linear optical approaches and time-resolved imaging to take snapshots of complex chemical and biochemical phenomena, and to advance fundamental understanding. Computational chemistry is advancing improved methods for studying electronically excited states in molecules and extended mesoscale systems, which are critically important to the design of energy conversion processes and materials. Increasing emphasis is being placed on predictive modeling of chemical processes. Chemical physics research is emphasizing development of new theoretical and simulation techniques relevant to a wide variety of potential applications. Work is continuing on advanced combustion research to accelerate the predictive simulation of highly efficient and clean internal combustion engines.	Research will continue to develop and apply forefront ultrafast x-ray and optical probes of matter, utilizing the LCLS, BES synchrotron light sources, and table-top laser-based ultrafast light sources, all aimed to advance fundamental understanding. Concomitant advances in theoretical methods will be sought to guide and interpret ultrafast measurements and for predicting ultrafast phenomena. Increased emphasis will be placed on time-resolved x-ray probes of matter at unprecedented short time scales and in systems of substantial complexity. These will include non-linear x-ray phenomena, structural determinations for individual molecules and particles, and time-resolved imaging to record complex chemical and biochemical phenomena. Computational efforts will stress improved methods for electronically excited states in molecules and extended mesoscale systems, which are key to the efficient design of energy conversion processes and materials. Work will continue on advanced combustion research to accelerate the predictive simulation of highly efficient and clean internal combustion engines. Increased emphasis will be placed on investigating properties of combustion in high-pressure or multiphase systems.	Research support is flat compared to FY 2014. Efforts in predictive theory and modeling will be enhanced due to importance of such methods to guide and interpret increasingly complex measurements, and for predictive modeling of chemical processes. Studies of ultra cold molecules will be deemphasized and some well-developed research topics in molecular and particle spectroscopy may be redirected to evolving forefront areas.

FY 2014 Enacted	FY 2015 Request	Explanation of Changes FY 2015 vs. FY 2014 Enacted
Chemical Transformations Research		
Research is emphasizing the complementary development of computational methods for the simulation of photo-catalytic, fuel-forming reactions with efforts in synthesis and characterization of new catalytic materials that are designed at the nanoscale to function on the mesoscale. The catalytic conversion of biomass to fuels and other chemical products is a major emphasis. Novel approaches to the separation of carbon dioxide from post-combustion gas streams and oxygen from air prior to oxy-combustion and for research on the multi-scale dynamics of flow and plume migration in carbon sequestration, which can lead to improved models and risk assessment for carbon sequestration, are being explored. Actinide research in support of advanced nuclear energy systems is continuing, with emphasis on complex separation chemistry addressing the multiplicity of chemical forms and oxidation states in actinides for nuclear fuels and waste forms.	Research will continue in the development of computational and complementary synthesis and atomic-level characterization for discovery of catalytic mechanisms enabling design of materials at the nanoscale for new or enhanced photo-catalytic and fuel-forming chemistries. The catalytic conversion of biomass to fuels and other energy related chemical products will be emphasized. The discovery and design of novel separation approaches to carbon dioxide capture from post-combustion gas streams and oxygen from air prior to oxy-combustion will continue with added integration with computational methods. Research will continue on the multi-scale dynamics of reactive flow and plume migration in subsurface reservoirs, which can lead to improved models and risk assessment for carbon sequestration and other subsurface applications. Actinide research in support of advanced nuclear energy systems will continue, with emphasis on new insights in actinides chemical bonding enabling new chemistry for separation and related nuclear fuels and waste form processes. In support of the departmental emphasis on subsurface engineering, aspects of the separations and the geosciences portfolios will support new efforts in carbon capture and sequestration as well as research in geophysical characterization and monitoring techniques.	Research support is flat compared to FY 2014. Areas of increased emphasis include actinide chemical bonding and integration of computational and theoretical methods. Research in subsurface engineering complementary to applied efforts in the technology offices will be enhanced. Some mature areas of research in polymer synthesis, analytical mass spectrometry, and geophysics may be decreased.

FY 2014 Enacted	FY 2015 Request	Explanation of Changes FY 2015 vs. FY 2014 Enacted
Photochemistry and Biochemistry Research		
The development of computational methods for the simulation of light harvesting and conversion of solar energy into electricity and fuels is being emphasized (in coordination with the *Chemical Transformations* activity). Experimental research on direct conversion of solar energy to fuels and for advancing the catalytic conversion of biomass to fuels, both of which require translation from the nano to the mesoscale, is being supported. These include studies of the mechanisms that protect and self-repair the natural photosynthetic apparatus; photocatalytic generation of fuels in synthetic systems via semiconductor/polymer interfaces, dye-sensitized solar cells, inorganic-organic molecular complexes, and nano-scale water splitting assemblies; and advanced analysis of the structure of plant cell walls to elucidate catalytic routes for the conversion of biomass to fuels and other chemical products (in coordination with the *Chemical Transformations* activity).	Research on fundamental aspects of light energy capture and conversion in non-biological and biological (photosynthetic) systems will continue to be emphasized, providing a critical foundation for direct conversion of solar energy to electricity, fuels, and high-value chemicals. Enhanced support for computational and modeling studies will enable the design and fabrication of novel semiconductor/ polymer interfaces, dye-sensitized solar cells, inorganic-organic molecular complexes, and biohybrid light harvesting complexes. Greater emphases on understanding the mechanisms of water-splitting, redox, and other energy-relevant biological (enzymatic) reactions, from the nano- to the mesoscale, will provide new insights important for development of novel bio-inspired catalysts based on earth-abundant materials, while biosynthetic and structural studies of the plant cell wall will help inform catalytic strategies for the direct conversion of biomass to fuels and other products.	Research support is flat compared to FY 2014. Research related to mesoscale phenomena in natural systems will be enhanced. Efforts in molecular solar thermal energy storage and solar energy conversion in artificial membranes will be deemphasized. Research on plant developmental and stress response mechanisms targeted towards biomass production may also be decreased.

FY 2014 Enacted	FY 2015 Request	Explanation of Changes FY 2015 vs. FY 2014 Enacted
Energy Frontier Research Centers (EFRCs)		
A single Funding Opportunity Announcement (FOA) was issued for both renewal and new EFRCs for 5-year awards beginning in FY 2014. The EFRC FOA encouraged the formation of effective teams to address the broad range of fundamental science needed to power transformative energy technologies, including newly identified opportunities in the computational design of materials and chemical processes and mesoscale science. All current EFRCs, including those initially through ARRA, had the opportunity to compete for a second five-year performance period. All awards, both new and renewal, will be based on rigorous peer review of the research proposed for the five year award term. Applicants requesting renewal funding will also be assessed on progress during the first five-year award.	The EFRCs that will be started in FY 2014 will perform the first year of research of the award period as outlined in their proposals. This multidisciplinary research will continue to provide accelerated progress in fundamental, energy-use inspired research. The research in these new EFRCs includes investigations of mesoscale science and utilization of computational research to predictably design new materials and processes. BES will hold a peer review to assess management and early operations.	FY 2015 support for EFRCs will continue at the FY 2014 level.

FY 2014 Enacted	FY 2015 Request	Explanation of Changes FY 2015 vs. FY 2014 Enacted
Energy Innovation Hubs—Fuels From Sunlight		
In FY 2014, JCAP performance milestones emphasize prototype development to test components for the integrated system. Areas of increased emphasis include analysis of components, materials and chemical inputs, and hardware designs with respect to manufacturability, life-cycle costs, and reusability to ensure the scalability of the first-generation, solar fuels generation system. Additional efforts are being made to fully optimize catalyst and systems efficiencies and to provide reviews of solar fuels research to the scientific community, establishing strong outreach efforts focused on workforce development necessary for development of a solar fuels industry.	The Fuels from Sunlight Hub completes its 5-year award at the planned level. Decision for continued funding beyond the 5 year term, which ends in September 2015, will be made in FY 2015.	The funding is approximately flat compared to FY 2014. A decision for continued funding beyond the initial five-year award term, which ends in September 2015, will be made in FY 2015.
General Plant Projects		
Funding is supporting minor facility improvements at Ames Laboratory.	Funding will support minor facility improvements at Ames Laboratory.	GPP support is flat compared to FY 2014.

Description

The Scientific User Facilities subprogram supports the operation of a geographically diverse suite of major facilities that provide thousands of researchers from universities, industry, and government laboratories 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 many disciplines from academia, national laboratories, and industry to utilize the facilities' unique capabilities and sophisticated instrumentation.

Studying matter at the level of atoms and molecules requires instruments that can probe structures that are one thousand times smaller than those detectable by the most advanced light microscopes. Thus, to characterize structures with atomic detail, we must use probes such as x-rays, electrons, and neutrons that are at least as small as the structures being investigated. The BES large-scale user facilities portfolio consists of a complementary set of intense x-ray sources, neutron scattering centers, and research centers for nanoscale science. These facilities allow researchers to probe materials in space, time, and energy with the appropriate resolutions that can interrogate the inner workings of matter to answer some of the most challenging grand science questions. By 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.

Advances in tools and instruments often drive scientific discovery. The continual development and upgrade of the instrumental capabilities include new x-ray and neutron experimental stations, improved core facilities, and new stand-alone instruments. The subprogram also supports research in accelerator and detector development to explore technology options for the next generations of x-ray and neutron sources.

Annually, the BES scientific facilities are used by more than 15,000 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. Collectively, these user facilities and enabling tools contribute to 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 enable scientific insights that can lead to the discovery and design of advanced materials and novel chemical processes with broad societal impacts, from energy applications to information technologies and biopharmaceutical discoveries. The advances enabled by these facilities extend from energy-efficient catalysts for clean energy production to spin-based electronics and new drugs for cancer therapy. For approved, peer-reviewed projects, operating time is available without charge to researchers who intend to publish their results in the open literature.

Synchrotron Radiation Light Sources

X-rays are an essential tool for studying the structure of matter and have long been used to peer into material through which visible light cannot penetrate. Today's synchrotron light source facilities produce x-rays that are billions of times brighter than medical x-rays. Scientists use these highly focused, intense beams of x-rays to reveal the identity and arrangement of atoms in a wide range of materials. The tiny wavelength of x-rays allows us to see things that visible light cannot resolve, such as the arrangement of atoms in metals, semiconductors, biological molecules, and other materials. The fundamental tenet of materials research is that structure determines function. The practical corollary that converts materials research from an intellectual exercise into a foundation of our modern technology-driven economy is that structure can be manipulated to construct materials with particular desired behaviors. To this end, synchrotron radiation has transformed the role of x-rays as a mainline tool for probing the atomic and electronic structure of materials internally and on their surfaces.

From its first systematic use as an experimental tool in the 1960s, synchrotron radiation has vastly enhanced the utility of pre-existing and contemporary techniques, such as x-ray diffraction, x-ray spectroscopy, and imaging and has given rise to scores of new ways to do experiments that would not otherwise be feasible with conventional x-ray machines. Moreover, the wavelength can be selected over a broad range (from the infrared to hard x-rays) to match the needs of particular experiments. Together with additional features, such as controllable polarization, coherence, and ultrafast pulsed time structure, these characteristics make synchrotron radiation the x-ray source of choice for a wide range of materials research. 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.

BES operates a suite of five light sources, including a free electron laser, the Linac Coherent Light Source (LCLS) at SLAC National Accelerator Laboratory (SLAC) and four storage ring based light sources—the Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory (LBNL), Advanced Photon Source (APS) at Argonne National Laboratory (ANL), Stanford Synchrotron Radiation Lightsource (SSRL) at SLAC, and the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory (BNL), which will cease operation in FY 2015. NSLS-II will transition from early operations to full operations during FY 2015. Funds are provided to support facility operations, enable cutting-edge research 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 user proposals.

<u>High Flux Neutron Sources</u>

One of the goals of modern materials science is to understand the factors that determine the properties of matter on the atomic scale and to use this knowledge to optimize those properties or to develop new materials and functionality. This process regularly involves the discovery of fascinating new physics, which itself may lead to previously unexpected applications. Among the different probes used to investigate atomic-scale structure and dynamics in scattering experiments, thermalized neutrons have unique advantages:

- they have a wavelength similar to the spacing between atoms, allowing atomic resolution studies of structure and have an energy similar to the elementary excitations of atoms and magnetic spins in materials, thus allowing an investigation of material dynamics;
- they have no charge, allowing deep penetration into a bulk material;
- they are scattered to a similar extent by both light and heavy atoms but differently by different isotopes of the same element, so that different chemical sites can be distinguished via isotope substitution experiments, for example in organic and biological materials;
- they have a magnetic moment, and thus can probe magnetism in condensed matter systems; and
- their scattering cross-section is precisely measurable on an absolute scale, facilitating straightforward comparison with theory and computer modeling.

The High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory (ORNL) generates neutrons via fission in a research reactor. HFIR operates at 85 megawatts and provides state-of-the-art facilities for neutron scattering, materials irradiation, and neutron activation analysis. It is the world's leading production source of elements heavier than plutonium for medical, industrial and research applications. There are 13 neutron scattering instruments installed in the reactor hall at HFIR and the adjacent new cold neutron beam guide hall and include world-class inelastic scattering spectrometers, small angle scattering, powder and single crystal diffractometers, neutron imaging, and an engineering diffraction machine.

Another approach for generating neutron beams is to use an accelerator to generate protons that strike a heavy-metal target. As a result of the impact, neutrons are produced in a process known as spallation. The Spallation Neutron Source (SNS) at ORNL is the world's brightest pulsed neutron facility and presently includes 16 instruments. These instruments include very high resolution inelastic and quasi-elastic scattering capabilities, powder and single crystal diffraction, polarized and unpolarized beam reflectometry, spin echo and small angle scattering spectrometers. A full suite of high and low temperature, high magnetic field, and high pressure sample environment equipment is available on each instrument. These neutron instruments are in high demand by researchers world-wide in a range of disciplines from biology to materials sciences and condensed matter physics.

The Lujan Neutron Scattering Center at Los Alamos National Laboratory (LANL), a pulsed spallation source operating at about 100 kW, supports a target hall constructed by the Office of Science and instruments developed by SC and the National Nuclear Security Administration that address both of the needs of the basic research community and the NNSA mission of science-based stockpile stewardship. The seven BES-supported instruments focused primarily on powder diffraction, local structure determinations, liquids and polarized-beam reflectometry, and engineering diffraction. The neutron flux at the Lujan Center is an order of magnitude below what is available at the SNS. In FY 2015, BES operations at the Lujan Neutron Scattering Center will cease and funding is requested to transition the facility to a safe storage condition.

Nanoscale Science Research Centers (NSRCs)

Nanoscience is the study of materials and their behaviors at the nanometer scale—probing single atoms, clusters of atoms, and molecular structures. The scientific quest is to design, observe, and understand how nanoscale structures function, including how they interact with their environment. Developments at the nanoscale have the potential to make major contributions to delivering remarkable scientific discoveries that transform our understanding of energy and matter and advance national, economic, and energy security.

The NSRCs are DOE’s premier user facilities for interdisciplinary research at the nanoscale, serving as the basis for a national program that encompasses new science, new tools, and new computing capabilities. The five NSRCs are the Center for Nanoscale Materials at ANL, Center for Functional Nanomaterials at BNL, Molecular Foundry at LBNL, Center for Nanophase Materials Sciences at ORNL, and Center for Integrated Nanotechnologies at SNL and LANL. Each center has particular expertise and capabilities, such as synthesis of nanomaterials; theory, modeling and simulation; imaging and spectroscopy including electron microscopy; and nanoscale integration. Selected thematic areas include catalysis, electronic materials, nanoscale photonics, and soft and biological materials. The centers are housed in 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. Operating funds are provided to enable cutting-edge research and technical support and to administer a robust user program at these facilities, which are made available to all researchers with access determined through external peer review of user proposals.

In FY 2015, the three electron-beam microcharacterization centers (EBMCs) will be merged administratively with their respective neighboring NSRCs. The three centers that will be merged are the Electron Microscopy Center for Materials Research at ANL, the National Center for Electron Microscopy at LBNL, and the Shared Research Equipment user facility at ORNL. The EBMCs provide superior spatial resolution and the ability to simultaneously obtain structural, chemical, and other types of information from sub-nanometer regions.

Other Project Costs

The total project cost (TPC) of DOE’s construction projects comprises two major components—the total estimated cost (TEC) and other project costs (OPC). The TEC includes project costs incurred after Critical Decision-1, such as costs associated with all engineering design and inspection, the acquisition of land and land rights; direct and indirect construction/fabrication; and the initial equipment necessary to place the facility or installation in operation; and facility construction costs and other costs specifically related to those construction efforts. OPC represents all other costs related to the projects that are not included in the TEC. Generally, other project costs are 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. OPC is always funded via operating funds.

Major Items of Equipment

BES supports major item of equipment (MIE) projects to ensure the continual development and upgrade of major scientific instrument capabilities, including fabricating new x-ray and neutron experimental stations, improving core facilities, and providing new stand-alone instruments. In general, each MIE greater than $5,000,000 in total project cost and all line item construction projects follow the DOE Project Management Order 413.3B, which requires formal reviews to obtain critical decisions that advance the development stages of a project. Additional reviews may be required depending on the complexity and needs of the projects in question. BES MIE projects are in two main categories: Synchrotron Radiation Light Sources and High Flux Neutron Sources.

Research

This activity supports targeted basic research in accelerator physics, x-ray and neutron detectors, and developments of advanced x-ray optics. Accelerator research is the cornerstone for the development of new technologies that will improve performance of accelerator-based light sources and neutron scattering facilities. Research areas include ultrashort pulse free electron lasers (FELs), new seeding techniques and other optical manipulation to reduce the cost and complexity and improve performance of next generation FELs, and very high frequency laser photoinjectors that can influence the design of linac-based FELs with high repetition rates. Detector research is a crucial component to enable the optimal utilization of user facilities, together with the development of innovative optics instrumentation to advance photon-based sciences, and data management techniques. The emphasis of the detector activity is on research leading to new and more efficient photon and neutron detectors. Research includes studies on creating, manipulating, transporting, and performing diagnostics of ultrahigh brightness beams.

This activity also supports long term surveillance and maintenance (LTS&M) responsibilities and legacy cleanup work at Brookhaven National Laboratory and SLAC National Accelerator Laboratory. Prior to FY 2014, this activity was funded by the DOE Environmental Management (EM) program.

This activity historically supported the three electron-beam microcharacterization centers (EBMCs). Starting in FY 2015, each EBMC will be merged administratively with their respective neighboring NSRCs.

Activities and Explanation of Changes

FY 2014 Enacted	FY 2015 Request	Explanation of Changes FY 2015 vs. FY 2014 Enacted
Synchrotron Radiation Light Sources		
The FY 2014 appropriation continues the early operations of the NSLS-II in addition to supporting the operations of the five BES light source facilities at an average of about 97% of optimal levels.	In FY 2015, funding is requested for operations of the light sources at optimal levels, including early operations for the newly constructed NSLS-II. NSLS will cease operations and funds are provided to transition the facility to a safe storage condition in FY 2015.	Increases in funding allow for operations of ALS, APS, SSRL and LCLS at their optimal level. The National Synchrotron Light Source (NSLS) will cease operations. The NSLS-II will transition from a construction project to operations in FY 2015.
High-Flux Neutron Sources		
Funding is provided to continue the operation of HFIR and SNS at an average of about 97% of optimal levels. The Los Alamos Neutron Science Center (LANSCE) is undergoing an upgrade which reduces operations of the Lujan Center to 2,000 hours.	Funding is requested to continue the operation of HFIR and SNS at optimal levels. The BES operations at the Lujan Neutron Scattering Center will cease and funding is requested to transition the facility to a safe storage condition.	The increase in funding allows for optimal operations of HFIR and SNS. Decreased funding for the Lujan Center will transition the facility to a safe storage condition.
Nanoscale Science Research Centers		
Funding is provided to continue operations and support of users at the NSRCs at an average of about 97% of optimal levels. Continued emphasis will be to cultivate and expand the user base from universities, national laboratories, and industry.	Funding will continue operations and support of users at the NSRCs at the optimal level. The electron-beam microcharacterization centers (EBMCs) are merged with the NSRCs in FY 2015. Continued program emphasis will be to cultivate and expand the user base from universities, national laboratories, and industry. Efforts will include planning for future electron scattering needs that could address scientific roadblocks toward observing ultrafast chemical and physical phenomena at ultra-small size scales in different sample environments.	Increases in funding are due to the merger of the EBMCs with the NSRCs as well as improved operational levels.

FY 2014 Enacted	FY 2015 Request	Explanation of Changes FY 2015 vs. FY 2014 Enacted
Other Project Costs		
Funds are provided in FY 2014 for Other Project Costs associated with the NSLS-II project at BNL and the LCLS-II project at SLAC according to the project plan.	Funds are requested in FY 2015 for Other Project Costs associated with the LCLS-II project at SLAC according to the project plan.	NSLS-II OPC is decreased by $27,400,000 according to the project plan. LCLS-II OPC is decreased by $700,000.
Major Items of Equipment		
Plans for APS-U continue to evolve, taking the findings and recommendations of the July 25, 2013 BES Advisory Committee report into account. APS-U begins conceptual planning related to implementation of the multi-bend achromat lattice and starts limited prototyping activities.	APS-U will continue with planning and design, prototyping, and research and development related to implementation of the multi-bend achromat lattice during FY 2015.	APS-U funding is flat with FY 2014.
NEXT is anticipated to receive CD-3 approval in 3Q FY 2014. The project continues design and procurements (long lead and regular), and begins construction/fabrication activities during FY 2014.	NEXT will continue with the design, procurements, construction/fabrication, installation, testing and commissioning of equipment during FY 2015.	NEXT funding is decreased by $2,500.

FY 2014 Enacted	FY 2015 Request	Explanation of Changes FY 2015 vs. FY 2014 Enacted
Research		
Funding is provided to support optimal operations of the three electron beam microcharacterization centers. Research activities on FEL self-seeding and advanced accelerator methods continue. The accelerator physics and detector research is supported to maintain a balanced portfolio that continues to push the frontiers in accelerator and detector research. In anticipation of advances in source output flux and data volume, developments of advanced x-ray optics and data management techniques are necessary to fully realize advancements of accelerator and detector research. In FY 2014, responsibility is transferred from EM to BES for long term surveillance and maintenance (LTS&M) and for remaining legacy cleanup work scope at BNL and SLAC.	The research funding for the scientific user facilities is projected to maintain the FY 2014 level of effort in FY 2015, with modest increases to support selected, high-priority research activities. This funding increase will allow efforts in x-ray optics developments and data management techniques in addition to continue to support seminal advances in accelerator and detector research cognizant of the DOE mission needs and instrumentation relevant to neutron and photon based science. FY 2015 funding for the three Electron Beam Microcharacterization Centers (EBMCs) will be merged with the Nanoscale Science Research Centers (NSRCs) budget. Funding to continue the long term surveillance and maintenance responsibilities at BNL and SLAC is also included in this portion of the budget.	The funding for the three electron-beam micro characterization centers is moved to the Nanoscale Science Research Centers. Taking into account this change, research continues with a modest increase from the FY 2014 level, and includes additional efforts in x-ray optics developments and data management techniques.

Description

Reactors, accelerator-based x-ray light sources, and pulsed neutron sources are expensive but necessary user facilities that enable critical DOE mission-driven science. These user facilities provide the academic, laboratory, and industrial research communities with the tools to fabricate, characterize, and develop new materials and chemical processes to advance basic and applied research, advancing chemistry, physics, earth science, materials science, environmental science, biology, and biomedical science. Regular investments in construction of new user facilities and upgrades to existing user facilities are essential to maintaining U.S. leadership in these research areas.

The National Synchrotron Light Source-II (NSLS-II) construction project will complete construction and begin operations in FY 2015. NSLS-II will allow scientists to probe the fundamental properties of matter with nanometer-scale resolution and atomic sensitivity paving the way to new scientific discoveries and innovations. Taking the findings and recommendations of the July 25, 2013 BES Advisory Committee report into account, the Linac Coherent Light Source-II (LCLS-II) project will be modified to include the addition of a superconducting linear accelerator and additional undulators to generate an unprecedented high-repetition-rate free-electron laser. This new, world-leading, high-repetition-rate x-ray source will solidify the LCLS complex as the world leader in ultrafast x-ray science for decades to come.

All BES construction projects are conceived and planned with the scientific community and, during construction, adhere to the highest standards of safety and are executed on schedule and within cost through dogged project management. In accordance with DOE Order 413.3B, each project is closely monitored and must perform within 10% of the cost and schedule performance baselines, established at Critical Decision 2, Approve Performance Baseline, and which are reproduced in the construction project data sheet.

Activities and Explanation of Change

FY 2014 Enacted	FY 2015 Request	Explanation of Changes FY 2015 vs. FY 2014 Enacted
Linac Coherent Light Source-II (LCLS-II)		
LCLS-II continues work to incorporate design changes, taking into account the findings and recommendations of the July 25, 2013 BES Advisory Committee report. Funding is provided for planning and project baseline development, engineering design, prototyping, and research and development activities.	The project will continue with design, initiate critical long-lead procurements of technical materials and cryogenics, continue research and development and prototyping activities, and fabrication of technical equipment during FY 2015.	LCLS-II funding is increased by $63,000,000. The funding will enable advancement of research and development activities, long-lead procurements, and prototyping.
National Synchrotron Light Source-II (NSLS-II)		
Funding requested for the civil construction will be ramped down, as scheduled.	No construction funding is requested for NSLS-II in FY 2015.	FY 2014 is the last year of construction funding for NSLS-II.

Basic Energy Sciences
Performance Measures

In accordance with the GPRA Modernization Act of 2010, the Department sets targets for, and tracks progress toward, achieving performance goals for each program. For more information, refer to the Department's FY 2013 Annual Performance Report.

	FY 2013	FY 2014	FY 2015
Performance Goal (Measure)	**BES Facility Operations—Average achieved operation time of BES user facilities as a percentage of total scheduled annual operation time**		
Target	≥ 90%	≥ 90%	≥ 90%
Result	Met	TBD	TBD
Endpoint Target	Many of the research projects that are undertaken at the Office of Science's scientific user facilities take a great deal of time, money, and effort to prepare and regularly have a very short window of opportunity to run. If the facility is not operating as expected the experiment could be ruined or critically setback. In addition, taxpayers have invested millions or even hundreds of millions of dollars in these facilities. The greater the period of reliable operations, the greater the return on the taxpayers' investment.		
Performance Goal (Measure)	**BES Facility Construction/MIE Cost & Schedule—Cost-weighted mean percent variance from established cost and schedule baselines for major construction, upgrade, or equipment procurement projects.**		
Target	< 10%	< 10%	< 10%
Result	Met	TBD	TBD
Endpoint Target	Adhering to the cost and schedule baselines for a complex, large scale, science project is critical to meeting the scientific requirements for the project and for being good stewards of the taxpayers' investment in the project.		

	FY 2013	FY 2014	FY 2015
Performance Goal (Measure)	**BES Solar Fuels—Demonstrate a scalable solar-fuels generator using Earth-abundant elements that produces fuel (without wires) from the sun 10 times more efficiently than current agriculturally produced plants**		
Target	Establish benchmarking capabilities for comparison of homogeneous/heterogeneous catalysts and light absorbers under standardized testing conditions	Design first prototype device for testing components, such as catalysts, light harvesters, membranes, and interfaces, as an integrated system	N/A
Result	Met	TBD	TBD
Endpoint Target	Demonstration of a scalable solar-fuels generator using Earth-abundant elements that produces fuel (without wires) from the sun 10 times more efficiently than current agriculturally produced plants. The performance goal will be achieved by the *Fuels from Sunlight* Energy Innovation Hub.		

Performance Goal (Measure)	**BES Energy Storage—Deliver two high-performance research energy storage prototypes for transportation and the grid that project at the battery pack level to be five times the energy density at 1/5 the cost of the 2011 commercial baseline.**		
Target	N/A	N/A	Through the "electrolyte genome," demonstrate a framework for designing new electrolytes using structure-chemical trends extracted from >10,000 first-principles calculated molecular motifs, modifications and mutations
Result	N/A	N/A	TBD
Endpoint Target	Deliver two high-performance research prototypes for transportation and the grid that project at the battery pack level to be five times the energy density at 1/5 the cost of the 2011 commercial baseline. The performance goal will be achieved by the *Batteries and Energy Storage* Energy Innovation Hub.		

Basic Energy Science
Capital Summary ($K)

	Total	Prior Years	FY 2013 Current	FY 2014 Enacted	FY 2014 Current	FY 2015 Request	FY 2015 vs. FY 2014 Enacted
Capital Operating Expenses Summary							
Capital Equipment	n/a	n/a	75,931	50,100	50,100	44,500	-5,600
General Plant Projects (GPP)	n/a	n/a	7,000	600	600	600	0
Accelerator Improvement Projects (AIP)	n/a	n/a	9,050	9,000	9,000	13,475	+4,475
Total, Capital Operating Expenses	n/a	n/a	91,981	59,700	59,700	58,575	-1,125
Capital Equipment							
Major Items of Equipment							
Advanced Photon Source Upgrade (APS-U), ANL (TPC TBD)	TBD[a]	20,000	20,000	20,000	20,000	20,000	0
Linac Coherent Light Source-II (LCLS-II), SLAC	—[b]	44,500[c]	22,500[d]	0[b]	0[b]	0[b]	0
NSLS-II Experimental Tools (NEXT), BNL (TPC $90,000)	90,000	15,000	12,000	25,000	25,000	22,500	-2,500
Total, Major Items of Equipment	**n/a**	**n/a**	**54,500**	**45,000**	**45,000**	**42,500**	**-2,500**
Other capital equipment projects under $2 million TEC	n/a	n/a	21,431	5,100	5,100	2,000	-3,100
Total, Capital equipment	**n/a**	**n/a**	**75,931**	**50,100**	**50,100**	**44,500**	**-5,600**
General Plant Projects (GPP)							
Ames Sensitive Instrument Facility	9,900	5,500	4,400	0	0	0	0
Combustion Research Facility	9,200	8,250[e]	950	0	0	0	0
Other general plant projects under $5 million TEC	n/a	n/a	1,650	600	600	600	0
Total, General Plant Projects	n/a	n/a	7,000	600	600	600	0
Accelerator Improvement Projects (AIP)							
Accelerator improvement projects under $5 million TEC	n/a	n/a	9,050	9,000	9,000	13,475	+4,475

[a] Following the July 2013 BESAC report on Future X-Ray Light Sources, the APS-U project has been rescoped and a revised CD-0 document is in preparation.
[b] LCLS-II is requested as a line item construction project in FY 2014 and FY 2015.
[c] LCLS-II received $30,000,000 in FY 2012 as a MIE ($22,000,000 as TEC and $8,000,000 as OPC). FY 2012 funds in the amount of $22,500,000 were also provided to LCLS-II in FY 2013. Prior to FY 2014, LCLS-II was an MIE.
[d] FY 2013 funding was requested as a line item, but due to the Continuing Resolution, FY 2013 funds are executed as a MIE.
[e] $2,550,000 was provided by the Energy Efficiency and Renewable Energy program and Sandia National Laboratories.

Major Items of Equipment Descriptions

Advanced Photon Source Upgrade (APS-U)

The Advanced Photon Source Upgrade (APS-U) MIE supports 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). The APS is one of the Nation's most productive x-ray light source facilities, serving over 4,000 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 hard x-ray 7 GeV source in the U.S. and only one of four in the world, along with the European Synchrotron Radiation Facility (ESRF) in France, PETRA-III in Germany, and Spring-8 in Japan. High-energy penetrating x-rays are especially critical for probing materials under real working environments, such as a battery or fuel cell in action. All three foreign facilities are well into campaigns of major upgrades of beamlines and also incorporating technological advancements in accelerator science. With the ever increasing demand for higher penetration power for probing real-world materials and applications, the higher energy hard x-rays (20 keV and above) produced at APS provide unique capabilities in the U.S. arsenal needed for tackling the grand science and energy challenges of the 21st Century. In response to the findings and recommendations of the July 25, 2013 BES Advisory Committee report, the APS-U Project will upgrade the existing APS to provide scientists with an x-ray source possessing world-leading transverse coherence and extreme brightness. The magnetic lattice of the APS storage ring will be upgraded to a multi-bend achromat configuration to provide brightness enhancements. The APS upgrade will ensure that the APS remains a world leader in hard x-ray science. The high-energy penetrating x-rays will provide a unique scientific capability directly relevant to problems in energy, the environment, new and improved materials, and biological studies. The upgraded APS will complement the capabilities of the 4th generation light sources (e.g., the Linac Coherent Light Source and Linac Coherent Light Source-II), which occupy different spectral, flux, and temporal range of technical specifications. The project is managed by Argonne National Laboratory.

NSLS-II Experimental Tools (NEXT)

The NSLS-II Experimental Tools (NEXT) MIE supports activities to add beamlines to the National Synchrotron Light Source-II (NSLS-II) Project. 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 operation of NSLS-II. The project is managed by Brookhaven National Laboratory.

Construction Projects Summary ($K)

	Total	Prior Years	FY 2013 Current	FY 2014 Enacted	FY 2014 Current	FY 2015 Request	FY 2015 vs. FY 2014 Enacted
13-SC-10, Linac Coherent Light Source-II (LCLS-II), SLAC							
TEC	846,400	0[a]	0[b]	75,700	75,700	138,700	+63,000
OPC	48,600	10,600	0	10,000	10,000	9,300	-700
TPC	**895,000**	**10,600**	**0**	**85,700**	**85,700**	**148,000**	**+62,300**
07-SC-06, National Synchrotron Light Source-II, BNL							
TEC	791,200	717,697	47,203	26,300	26,300	0	-26,300
OPC	120,800	69,000	24,400	27,400	27,400	0	-27,400
TPC	**912,000**	**786,697**	**71,603**	**53,700**	**53,700**	**0**	**-53,700**
Total, Construction							
TEC	n/a	n/a	47,203[b]	102,000	102,000	138,700	+36,700
OPC	n/a	n/a	24,400	37,400	37,400	9,300	-28,100
TPC	**n/a**	**n/a**	**71,603**	**139,400**	**139,400**	**148,000**	**+8,600**

Funding Summary ($K)

	FY 2013 Current	FY 2014 Enacted	FY 2015 Request	FY 2015 vs. FY 2014 Enacted
Research	676,085	698,962	711,250	+12,288
Scientific User Facilities Operations	743,118	778,785	851,454	+72,669
Major Items of Equipment	54,500	45,000	42,500	-2,500
Construction Projects (includes OPC)	71,603	139,400	148,000	+8,600
Other[c]	5,950	49,782	53,296	+3,514
Total, Basic Energy Sciences	**1,551,256**	**1,711,929**	**1,806,500**	**+94,571**

[a] LCLS-II received $30,000,000 in FY 2012 as an MIE ($22,000,000 as TEC and $8,000,000 as OPC). FY 2012 funds in the amount of $22,500,000 were also provided to LCLS-II in FY 2013.

[b] FY 2013 funding was requested as a line item, but due to a Continuing Resolution, $22,500,000 in FY 2013 was executed as an MIE.

[c] Includes SBIR/STTR funding and non-Facility related GPP.

Facility Operations ($K)

	FY 2013 Current	FY 2014 Enacted	FY 2015 Request	FY 2015 vs. FY 2014 Enacted
Advanced Light Source	$59,500	$60,000	$63,307	+$3,307
Achieved operating hours	4,891	N/A	N/A	
Planned operating hours	4,700	5,100	5,600	+500
Optimal hours	4,800[a]	5,300[b]	5,600	+300
Percent of optimal hours	101.9%	96.2%	100.0%	
Unscheduled downtime percentage	<10%	<10%	<10%	
Number of users	2,222	1,800	2,000	+200
Advanced Photon Source	$120,170	$123,000	$129,852	+$6,852
Achieved operating hours	4,895	N/A	N/A	
Planned operating hours	5,000	5,000	5,000	0
Optimal hours	5,000	5,000	5,000	0
Percent of optimal hours	97.9%	100%	100%	
Unscheduled downtime percentage	<10%	<10%	<10%	
Number of users	4,542	4,500	4,600	+100
National Synchrotron Light Source, BNL	$33,000	$30,000	$5,500	-$24,500
Achieved operating hours	5,538	N/A	N/A	
Planned operating hours	4,500	4,400	0	-4,400
Optimal hours	4,500[a]	4,500[b]	0	-4,500
Percent of optimal hours	123.1%	97.8%	0	
Unscheduled downtime percentage	<10%	<10%	0	
Number of users	2,367	1,500	0	-1,500
National Synchrotron Light Source-II, BNL	$22,000	$56,000	$115,000	+$59,000
Achieved operating hours	N/A	N/A	N/A	N/A
Planned operating hours	0	0	2,500	+2,500
Optimal hours	0	0	2,500	+2,500
Percent of optimal hours	0	0	100%	0

[a] The optimal hours for ALS are adjusted from 5,600 to 4,800 hours in FY 2013 and 5,600 to 5,300 hours in FY 2014 to allow for installation of new hardware and maintenance activities.

[b] The optimal hours for NSLS are adjusted from 5,400 to 4,500 hours in FY 2013 and FY 2014 as part of the transition plan for ramping down NSLS operations.

	FY 2013 Current	FY 2014 Enacted	FY 2015 Request	FY 2015 vs. FY 2014 Enacted
Unscheduled downtime percentage	0	0	<10%	0
Number of users	0	0	250	+250
Stanford Synchrotron Radiation Lightsource	$38,500	$38,500	$38,860	+$360
Achieved operating hours	5,160	N/A	N/A	
Planned operating hours	5,000	5,400	5,400	0
Optimal hours	5,200	5,400	5,400	0
Percent of optimal hours	99.2%	100%	100%	
Unscheduled downtime percentage	<10%	<10%	<10%	
Number of users	1,675	1,500	1,500	0
Linac Coherent Light Source	$123,000	$124,500	$131,647	+$7,147
Achieved operating hours	4,580	N/A	N/A	
Planned operating hours	4,100	4,400	4,500	+100
Optimal hours	4,500	4,500	4,500	0
Percent of optimal hours	101.8%	97.8%	100%	
Unscheduled downtime percentage	<10%	<10%	<10%	
Number of users	594	500	550	+50
High Flux Isotope Reactor	$58,000	$58,000	$60,030	+$2,030
Achieved operating hours	3,629	N/A	N/A	
Planned operating hours	3,300	3,400	3,500	+100
Optimal hours	3,400	3,500	3,500	0
Percent of optimal hours	106.7%	97.1%	100%	
Unscheduled downtime percentage	<10%	<10%	<10%	
Number of users	395	400	450	+50
Lujan Neutron Scattering Center	$10,000	$8,900	$2,000	-$6,900
Achieved operating hours	1,597	N/A	N/A	
Planned operating hours	3,000	1,300	0	-1,300
Optimal hours	3,000	2,000[a]	0	-2,000
Percent of optimal hours	53.2%	65.0%		
Unscheduled downtime percentage	<10%	<10%		

[a] The optimal hours for Lujan are adjusted from 3,000 to 2,000 hours in FY 2014 reflecting limited availability of LANSCE.

	FY 2013 Current	FY 2014 Enacted	FY 2015 Request	FY 2015 vs. FY 2014 Enacted
Number of users	208	150	0	-150
Spallation Neutron Source	$178,448	$179,000	$186,460	+$7,460
Achieved operating hours	4,270	N/A	N/A	
Planned operating hours	4,200	4,400	4,500	+100
Optimal hours	4,500	4,500	4,500	0
Percent of optimal hours	94.9%	97.8%	100%	
Unscheduled downtime percentage	<10%	<10%	<10%	
Number of users	726	750	800	+50
Center for Nanoscale Materials[a]	$20,050	$20,100	$24,405	+$4,305
Number of users	454	400	500	+100
Center for Functional Nanomaterials[a]	$19,550	$19,600	$20,700	+$1,100
Number of users	439	400	400	0
Molecular Foundry[a]	$20,050	$20,150	$27,614	+$7,464
Number of users	451	400	500	+100
Center for Nanophase Materials Sciences[a]	$20,300	$20,350	$24,344	+$3,994
Number of users	467	400	500	+100
Center for Integrated Nanotechnologies[a]	$20,550	$20,685	$21,735	+$1,050
Number of users	447	400	400	0
Total, All Facilities	$743,118	$778,785	$851,454	+$72,669
Achieved operating hours	34,560	N/A	N/A	
Planned operating hours	33,800	33,400	31,000	-2,400
Optimal hours	34,900	34,700	31,000	-3,700
Percent of optimal hours (funding weighted)	99.7%	97.7%	100.0%	
Unscheduled downtime percentage	0%	<10%	<10%	
Number of users	14,987	13,100	12,450	-650

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

Scientific Employment

	FY 2013 Estimate	FY 2014 Estimate	FY 2015 Estimate	FY 2015 vs. FY 2014
Number of permanent Ph.D.'s (FTEs)	4,680	4,450	4,490	+40
Number of postdoctoral associates (FTEs)	1,310	1,170	1,160	-10
Number of graduate students (FTEs)	2,050	1,740	1,730	-10

13-SC-10, Linac Coherent Light Source-II
SLAC National Accelerator Laboratory, Menlo Park, California
Project is for Design and Construction

1. Summary and Significant Changes

The Linac Coherent Light Source-II (LCLS-II) was initially designated as a major item of equipment (MIE). The FY 2013 request proposed funding LCLS-II as a construction project, but FY 2014 is the first year that construction project funding was appropriated. The FY 2015 LCLS-II project data sheet (PDS) shows both MIE and construction funding in order to convey the full scope of the project's funding. The LCLS-II project described in this PDS is a significant revision to the project described in previous years.

In January 2013, the Director of the Office of Science (SC) charged the BESAC to assess the Grand Science Challenges that could best be explored with current and possible future SC light sources and to provide light source specifications that would maximize their impact. A 22-member BESAC subcommittee used prior BESAC reports and new input from the x-ray sciences communities to formulate findings and recommendations. In July 2013, BESAC accepted the "Report of the BESAC Subcommittee on Future X-ray Light Sources" and delivered to the Office of Science their findings and recommendations, which are formulated to ensure that the U.S. maintains its preeminence in the critically important field of x-ray science by providing the U.S. x-ray user community with world leading performance from its free electron laser (FEL) and storage ring based x-ray sources.

Based on this report, the Office of Science directed the SLAC National Accelerator Laboratory (SLAC) to assess whether and how the BESAC recommendations could be incorporated into the LCLS-II project. The discussions that ensued resulted in the updated LCLS-II project presented here, which will build upon the exceptional characteristics of the LCLS for the production of hard x-rays and incorporate superconducting linear accelerator technology to enable high repetition rate operation up to 5 keV photon energies. The revised LCLS-II project will have the broadest photon energy range and the highest energy per pulse, and it will be the only high repetition rate FEL in the world. It will provide unprecedented x-ray properties for the combined control of spatial, temporal, and energy resolution that will enable groundbreaking research in a wide range of scientific disciplines.

The revised preliminary Total Project Cost (TPC) range supporting the recent BESAC recommendations and proposed technical approach is $750,000,000–$1,200,000,000. Prior to the BESAC recommendations, the most recent DOE 413.3B approved Critical Decision, CD-3A (Approve Long Lead Procurement (LLP) Baseline and Start of LLP), was approved on March 14, 2012. The preliminary TPC range for the project at that time was $350,000,000–$500,000,000. The addition of the superconducting linac and the cryogenic systems to enable the high repetition rate account for the cost increase.

The Mission Need Statement has been updated. The Acquisition Strategy is being revised to support the new technical approach. The cost estimate and range are being refined based upon the new technical strategy. The project will seek new long lead procurement authorization supporting the revised technical strategy as detailed requirements are refined.

A Federal Project Director has been assigned to this project and is certified to Level 4.

This PDS is not a new start for the FY 2015 budget year.

This PDS is an update of the FY 2014 proposal.

2. Critical Decision (CD) and D&D Schedule

(fiscal quarter or date)

	CD-0	CD-1	Design Complete	CD-2	CD-3A	CD-3B	CD-4	D&D
FY 2013	4/22/2010	10/14/2011	4Q FY 2016	1Q FY 2013	3/14/2012	3Q FY 2013	4Q FY 2019	N/A
FY 2014	4/22/2010	10/14/2011	4Q FY 2016	4Q FY 2013	3/14/2012	4Q FY 2013	4Q FY 2019	N/A
FY 2015	4/22/2010	10/14/2011	4Q FY 2017[a]	4Q FY 2015[a]	3/14/2012[a]	4Q FY 2016[a]	4Q FY 2021[a]	N/A

CD-0 – Approve Mission Need
CD-1 – Approve Alternative Selection and Cost Range
CD-2 – Approve Performance Baseline
CD-3A – Approve Long-Lead Procurements
CD-3 – Approve Start of Construction
CD-4 – Approve Start of Operations or Project Closeout

3. Baseline and Validation Status

(dollars in thousands)

	TEC, Design	TEC, Construction	TEC, Total	OPC, Except D&D	OPC, D&D	OPC, Total	TPC
FY 2013	18,000	367,000	385,000	20,000	0	20,000	405,000
FY 2014[a]	18,000	367,000	385,000	20,000	0	20,000	405,000
FY 2015[a]	47,000[b]	799,400[b]	846,400	48,600	0	48,600[b]	895,000[b]

4. Project Description, Scope and Justification

Mission Need

The LCLS-II project's purpose is to expand the x-ray spectral operating range and the user capacity of the existing Linac Coherent Light Source (LCLS) facility. The expanded spectral range will enable researchers to tackle new research frontiers. The capacity increase is critically needed as the demand for LCLS capabilities far exceeds the available time allocation to users. The revised LCLS-II presented in this PDS is informed by 2013 BESAC recommendations to provide "high repetition rate, ultra-bright, transform limited, femtosecond x-ray pulses over a broad photon energy (about 0.2–5 keV) with full spatial and temporal coherence" and the "linac should feed multiple independently tunable undulators each of which could have multiple endstations." Collectively, the project will enable groundbreaking research in a wide range of scientific disciplines in chemical, material and biological sciences.

Scope and Justification for 13-SC-10 Linac Coherent Light Source II

SLAC's advances in the creation, compression, transport, and monitoring of bright electron beams have spawned a new generation of x-ray radiation sources based on linear accelerators rather than on storage rings. The LCLS produces a high-brightness x-ray beam with properties vastly exceeding those of current x-ray sources in three key areas: peak brightness, coherence, and ultrashort pulses. The peak brightness of the LCLS is 10 billion times greater than current synchrotrons,

[a] This project is pre-CD-2; the estimated schedule is preliminary. Construction will not be executed without appropriate CD approvals.
[b] Includes MIE funding of $7,000,000 for the design phase and $60,000,000 for the construction phases, which results in $67,000,000 of TEC funding, as well as $18,600,000 of OPC funding, for a total of $85,600,000 of MIE funding in the TPC.

providing up to 10^{12} x-ray photons in a pulse with duration in the range of 3–500 femtoseconds. These characteristics of the LCLS have opened new realms of research in the chemical, material, and biological sciences. LCLS-II will build on the success of LCLS by expanding the spectral range of hard x-rays produced at the facility and adding a new high repetition rate, spectrally tunable x-ray source. The repetition rate for x-ray production in the 0.2–5 keV range will be increased by at least a factor of 1,000 to yield unprecedented high average brightness x-rays that will be unique worldwide.

LCLS is based on the existing SLAC linear accelerator (linac), which is not a superconducting linac. The linac was originally designed to accelerate electrons and positrons to 50 GeV for colliding beam experiments and for nuclear and high energy physics experiments on fixed targets and was later adapted for use as a FEL (the LCLS facility) and for advanced accelerator research. At present, the last third of the 3 kilometer linac is being used to operate the LCLS facility, and the first 2 kilometers are used for advanced accelerator research.

The initial LCLS-II project, described in the FY 2014 PDS, was to use the second kilometer of the linac to produce high-brightness (13.5 GeV) electron bunches at a 120 Hz repetition rate. These electron bunches would have been sent to a new undulator tunnel to produce two x-ray beams spanning a tunable photon energy range beyond the existing LCLS facility. Use of the first and third kilometers of the linac would have remained unchanged.

The revised LCLS-II project will construct a new high repetition rate electron injector and replace the first kilometer of the linac with a 4 GeV superconducting linac to create the electron beam required for x-ray production in the 0.2–5 keV range with a repetition rate near 1 MHz. The new electron beam will be transported to the existing undulator hall and will be capable of feeding either of the two new variable gap undulators.

The third kilometer of the linac will continue to produce 14 GeV electron bunches for hard x-ray production at a 120 Hz repetition rate. The electron bunches will be sent to both of the new undulators to produce two simultaneous x-ray beams. The x-ray beams will span a tunable photon energy range of 5 to 25 keV, beyond the range of the existing LCLS facility, and they will incorporate “self seeding sections” to greatly enhance the longitudinal coherence of the x-ray beams. The middle kilometer of the existing linac will not be used as part of LCLS-II but will continue to be used for advanced accelerator research and it would be available for future expansion of the LCLS-II capabilities.

At the completion of the LCLS-II project, the facility will operate two independent electron linacs and two independent x-ray sources, supporting up to six experiment stations. Both the capability and capacity of the facility will be significantly enhanced. The combined characteristics (spectral content, peak power, average brightness, pulse duration, and coherence) of the new x-ray sources will surpass the present capabilities of the LCLS beam in spectral tuning range and brightness. The high repetition rate will accommodate more experiments. Furthermore, the two new undulators will be independently controlled to enable more experiments to be conducted simultaneously.

Experience with LCLS has, for the first time, provided data on performance of the x-ray instrumentation and optics required for scientific experiments with the LCLS. The LCLS-II project will take advantage of this knowledge base to design LCLS-II x-ray transport, optics, and diagnostics matched to the characteristics of these sources. The LCLS-II project scope is able to leverage the existing suite of LCLS instrumentation for characterization of the x-ray sources with moderate upgrades primarily to address the higher repetition rate operation.

The existing LCLS Beam Transport and Undulator Hall will be modified as necessary to house the new undulators, electron beam dumps, and x-ray optics. The existing experimental stations will be updated as necessary for the exploitation of the new x-ray sources. In contrast to the initial version of the project, construction of a new undulator tunnel and a new instrument suite will not be required.

The LCLS-II project will develop strategic partnerships with other SC laboratories for the design, fabrication, installation, and commissioning of the new superconducting linear accelerator, the high repetition rate electron injector and the new variable gap undulators.

Funding for conceptual design in FY 2011 supported the creation of the initial facility concept. The project initiated engineering design and long lead procurements in FY 2012 as an MIE. FY 2013 funding continued long lead procurements, design of technical equipment, R&D, and prototyping of key technical components. FY 2014 funding continues design work, critical long-lead procurements of technical materials and cryogenics, R&D, prototyping activities, and fabrication of technical equipment. The Mission Need Statement has been updated. An updated Acquisition Strategy is being developed. FY 2015 activities will include design, long lead procurements, R&D, prototyping, construction/fabrication, and installation activities.

Key Performance Parameters (KPPs)

The Threshold KPPs, which will define the official performance baseline at CD-2, represent the minimum acceptable performance that the project must achieve. Achievement of the Threshold KPPs will be a prerequisite for approval of CD-4, Project Completion. The Objective KPPs represent the desired project performance. If project performance is sustained and funds are available, the project will strive to attain the Objective KPPs. The KPPs presented here are preliminary, pre-baseline values. The final key parameters will be established as part of CD-2, Performance Baseline.

Preliminary LCLS-II Key Performance Parameters

Performance Measure	Threshold	Objective
Variable gap undulators	2 (soft and hard x-ray)	2 (soft and hard x-ray)
Superconducting linac-based FEL system		
Superconducting linac electron beam energy	3 GeV	≥ 4 GeV
Superconducting linac repetition rate	50 kHz	1,000 kHz
Superconducting linac charge per bunch	0.02 nC	0.1 nC
Photon beam energy range	250–2,800 eV	200–5,000 eV
High repetition rate capable end stations	≥ 1	≥ 2
FEL photon quantity (10^{-3} BW[a])	10^{9} (10x spontaneous @ 2.5 keV)	> 10^{11} @ 2.5 keV
Normal conducting linac-based system		
Normal conducting linac electron beam energy	13 GeV	15 GeV
Normal conducting linac repetition rate	120 Hz	120 Hz
Normal conducting linac charge per bunch	0.1 nC	0.25 nC
Photon beam energy range	1–13,000 eV	1–25,000 eV
Low repetition rate capable end stations	≥ 2	≥ 3
FEL photon quantity (10^{-3} BW)	10^{10} (10x spontaneous @ 13 keV)	> 10^{12} @ 13 keV

[a] Fractional bandwidth. The specified KPPs are the number of photons with an energy within 0.1% of the specified central value.

5. Financial Schedule

	(dollars in thousands)		
	Appropriations	Obligations	Costs
Total Estimated Cost (TEC)			
Design phase			
MIE funding			
FY 2012	2,000[a]	2,000	2,000
FY 2013	5,000[b]	5,000	5,000
Total, MIE funding	7,000	7,000	7,000
Line item construction funding			
FY 2014	4,000	4,000	4,000
FY 2015	21,000	21,000	20,000
FY 2016	15,000	15,000	14,000
FY 2017	0	0	2,000
Total, Line item construction funding	40,000[c]	40,000	40,000
Total, Design phase	47,000	47,000	47,000
Construction phase			
MIE funding			
FY 2012	42,500[d]	20,000[a]	13,862
FY 2013	17,500[e]	40,000[a]	27,285
FY 2014	0	0	18,853
Total, MIE funding	60,000	60,000	60,000
Line item construction funding			
FY 2014	71,700	71,700	47,147
FY 2015	117,700	117,700	108,000
FY 2016	189,000	189,000	180,000
FY 2017	185,100	185,100	185,100
FY 2018	156,000	156,000	168,000
FY 2019	19,900	19,900	27,700

[a] FY 2012 funding was executed as an MIE. FY 2012 funding was used for design and long lead procurement.
[b] FY 2013 funding was requested as a line item, but due to a Continuing Resolution, FY 2013 funds were executed as an MIE.
[c] This project has not yet received CD-2 approval; funding estimates are preliminary.
[d] FY 2012 funding shown includes $22,500,000 of prior year balances from FY 2012 that was reallocated to the LCLS-II project during FY 2013.
[e] FY 2013 funding was requested as a line item, but due to a continuing resolution, FY 2013 funds were executed as a MIE.

(dollars in thousands)	Appropriations	Obligations	Costs
FY 2020	0	0	23,453
Total, Line item construction funding	739,400	739,400	739,400
Total, Construction phase	799,400	799,400	799,400
TEC			
MIE funding			
FY 2012	44,500[a]	22,000[a]	15,862
FY 2013	22,500[b]	45,000[a]	32,285
FY 2014	0	0	18,853
Total, MIE funding	67,000	67,000	67,000
Line item construction funding			
FY 2014	75,700	75,700	51,147
FY 2015	138,700	138,700	128,000
FY 2016	204,000	204,000	194,000
FY 2017	185,100	185,100	187,100
FY 2018	156,000	156,000	168,000
FY 2019	19,900	19,900	27,700
FY 2020	0	0	23,453
Total, Line item construction funding	779,400	779,400	779,400
Total, TEC	846,400[c]	846,400[c]	846,400[c]
Other Project Cost (OPC)			
OPC except D&D			
MIE funding			
FY 2010	1,126	1,126	938
FY 2011	9,474	9,474	8,033
FY 2012	8,000[a]	8,000	8,893
FY 2013	0	0	116
FY 2014	0	0	620
Total, MIE funding	18,600	18,600	18,600

[a] FY 2012 funding was executed as an MIE. FY 2012 funding was used for design and long lead procurement.
[b] FY 2013 funding was requested as a line item, but due to a Continuing Resolution, FY 2013 funds were executed as an MIE.
[c] This project has not yet received CD-2 approval; funding estimates are preliminary. Amounts shown include MIE funding of $67,000,000 in the TEC, $18,600,000 in the OPC, and $85,600,000 in the TPC.

	(dollars in thousands)		
	Appropriations	Obligations	Costs
Line item construction funding			
FY 2014	10,000	10,000	80
FY 2015	9,300	9,300	9,300
FY 2016	0	0	5,000
FY 2017	0	0	0
FY 2018	5,900	5,900	8,000
FY 2019	4,800	4,800	7,000
FY 2020	0	0	620
Total, Line item construction funding	30,000	30,000	30,000
Total, OPC	48,600[a]	48,600[a]	48,600[a]
Total Project Cost (TPC)			
MIE funding			
FY 2010	1,126	1,126	938
FY 2011	9,474	9,474	8,033
FY 2012	52,500[b]	30,000	24,755
FY 2013	22,500[c]	45,000	32,401
FY 2014	0	0	19,473
Total, MIE funding	85,600	85,600	85,600
Line item construction funding			
FY 2014	85,700	85,700	51,227
FY 2015	148,000	148,000	137,300
FY 2016	204,000	204,000	199,000
FY 2017	185,100	185,100	187,100
FY 2018	161,900	161,900	176,000
FY 2019	24,700	24,700	34,700
FY 2020	0	0	24,073
Total, Line item construction funding	809,400	809,400	809,400
Total, TPC	895,000[a]	895,000[a]	895,000[a]

[a] This project has not yet received CD-2 approval; funding estimates are preliminary. Amounts shown include MIE funding of $67,000,000 in the TEC, $18,600,000 in the OPC, and $85,600,000 in the TPC.

[b] FY 2012 funding shown includes $22,500,000 of prior year balances from FY 2012 that was reallocated to the LCLS-II project during FY 2013.

[c] FY 2013 funding was requested as a line item, but due to a continuing resolution, FY 2013 funds were executed as an MIE.

6. Details of Project Cost Estimate

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design			
Design	37,770	16,500	N/A
Contingency	9,230	1,500	N/A
Total, Design	47,000	18,000	N/A
Construction			
Site Preparation	4,700	4,700	N/A
Equipment	564,800	189,370	N/A
Other Construction	38,500	95,243	N/A
Contingency	191,400	77,687	N/A
Total, Construction	799,400[a]	367,000[a]	N/A
Total, TEC	846,400[a]	385,000[a]	N/A
Contingency, TEC	200,630	79,187	N/A
Other Project Cost (OPC)			
OPC except D&D			
Conceptual Planning	1,980	1,126	N/A
Conceptual Design	23,658	14,974	N/A
Research and Development	1,972	1,100	N/A
Start-Up	11,550	1,920	N/A
Contingency	9,440	880	N/A
Total, OPC	48,600[a]	20,000[a]	N/A
Contingency, OPC	9,440	880	N/A
Total, TPC	895,000[a]	405,000[a]	N/A
Total, Contingency	210,070	80,067	N/A

[a] This project has not yet received CD-2 approval; funding estimates are preliminary. Amounts shown include MIE funding of $67,000,000 in the TEC, $18,600,000 in the OPC, and $85,600,000 in the TPC, as detailed in table 5.

7. Schedule of Appropriations Requests

(dollars in thousands)

Request Year		Prior Years	FY 2012	FY 2013	FY 2014	FY 2015	FY 2016	FY 2017	FY 2018	FY 2019	Total
FY 2012 (MIE)	TEC	0	22,000	TBD	TBD	TBD	TBD	TBD	TBD	TBD	TBD
	OPC	10,600	8,000	TBD	TBD	TBD	TBD	TBD	TBD	TBD	TBD
	TPC	10,600	30,000	TBD	TBD	TBD	TBD	TBD	TBD	TBD	TBD
FY 2013 (MIE)[a]	TEC	0	22,000	63,500	80,300	94,000	105,300	19,900	0	0	385,000
	OPC	10,600	8,000	0	700	0	700	0	0	0	20,000
	TPC	10,600	30,000	63,500	81,000	94,000	106,000	19,900	0	0	405,000
FY 2014	TEC	0	22,000	—[b]	95,000	122,500	100,500	0	0	0	385,000
	OPC	10,600	8,000	—[b]	700	0	700	0	0	0	20,000
	TPC	10,600	30,000	—[b]	95,700	122,500	101,200	0	0	0	405,000
FY 2015	TEC	0	22,000	45,000	75,700	138,700	204,000	185,100	156,000	19,900	846,400[c]
	OPC	10,600	8,000	0	10,000	9,300	0	0	5,900	4,800	48,600[c]
	TPC	10,600	30,000	45,000	85,700	148,000	204,000	185,100	161,900	24,700	895,000[c]

8. Related Operations and Maintenance Funding Requirements

Not applicable. Project does not have CD-2 approval.

9. Required D&D Information

Area of existing facility being replaced and D&D'ed by this project:	N/A
Area of additional D&D space to meet the "one-for-one" requirement from the banked area:	All new construction has been offset by existing SLAC and DOE banked space.

10. Acquisition Approach

DOE has determined that the LCLS-II project will be acquired by the SLAC National Accelerator Laboratory under the existing DOE M&O contract.

A Conceptual Design Report for the LCLS-II project has been completed and will be revised based on the new technical parameters. Key design activities, requirements, and high-risk subsystem components will be identified to reduce cost and schedule risk to the project and expedite the startup. The necessary project management systems are fully up-to-date, operating, and are maintained as a SLAC-wide resource.

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[a] FY 2013 funding was requested as a line item construction project, but due to a continuing resolution, the project continued as an MIE.

[b] FY 2013 amounts in the FY 2014 budget request were not shown below the Congressional control level because a full-year appropriation had not yet been enacted when the budget was submitted. TEC, OPC, and TPC totals were based upon the FY 2013 request levels ($63,500,000 TEC and TPC and $0 OPC).

[c] This project has not yet received CD-2 approval; funding estimates are preliminary. Amounts shown include MIE funding of $67,000,000 in the TEC, $18,600,000 in the OPC, and $85,600,000 in the TPC, as detailed in table 5.

SLAC will partner with other SC laboratories for design and procurement of key technical subsystem components. Technical system designs will require research and development activities. Preliminary cost estimates for these systems are based on actual costs from LCLS, to the extent practicable. Recent cost data has been exploited fully in planning and budgeting for the project. Design of the technical systems will be completed by SLAC or partner laboratory staff. Technical equipment will either be fabricated in-house or subcontracted to vendors with the necessary capabilities.

All subcontracts will be competitively bid and awarded based on best value to the government. Project performance metrics for SLAC are included in the M&O contractor's annual performance evaluation and measurement plan.

Lessons learned in the LCLS Project are documented in its project completion report and will be exploited fully in planning and executing LCLS-II.