

## 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 investigate 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 2016 Budget Request

The FY 2016 Request for BES will support ongoing core research activities at or above the FY 2015 level with few exceptions for transitioning programs. Funding for the Batteries and Energy Storage Energy Innovation Hub will continue as planned. The Fuels from Sunlight Energy Innovation Hub is undergoing a review for a possible renewal for a final term with a maximum duration of five years; a renewal decision will be made in January 2015. Additional funding is requested for the Energy Frontier Research Centers (EFRCs) to invest in strategic areas of basic energy sciences that are not represented or are underrepresented in the current EFRC portfolio. The EFRC program will transition to a biennial solicitation cycle starting in FY 2016. The Computational Materials Sciences activity supports the second year of research awards that will be issued in FY 2015, and funds are requested for underrepresented research topics in predictive design of functional materials. A new investment in midscale instrumentation is also requested to develop cutting-edge electron scattering tools to advance the forefront of ultrafast science.

In FY 2016, BES will support near optimal operations of five x-ray light source facilities, two neutron source facilities, and five Nanoscale Science Research Centers. FY 2016 will be the first full year of operations for the newly constructed National Synchrotron Light Source-II (NSLS-II). No funds are requested for the National Synchrotron Light Source. The Linac Coherent Light Source-II project will ramp up construction activities, reaching its peak year of funding in FY 2016. The Advanced Photon Source Upgrade and the NSLS-II Experimental Tools (NEXT) major item of equipment projects will be supported as planned. FY 2016 is the last year of funding for the NEXT project.

DOE's subsurface cross-program crosscut, SubTER, aims to address identified challenges in the subsurface through highly focused and coordinated research in Wellbore Integrity, Stress State and Induced Seismicity, Permeability Manipulation, and New Subsurface Signals to ensure enhanced energy security, material impact on climate change via CO<sub>2</sub> sequestration, and dramatically mitigated environmental impacts from energy-related activities and operations. The BES contribution to SubTER will focus on fundamental geochemistry and geophysics with an emphasis on subsurface chemistry and complex fluid flow.

Over 80 percent of our total energy supply comes from the subsurface, and this importance is magnified by the ability to also use the subsurface to store and sequester fluids and waste products. SubTER will address identified challenges in the subsurface through highly focused and coordinated research in Wellbore Integrity, Stress State and Induced Seismicity, Permeability Manipulation, and New Subsurface Signals to ensure enhanced energy security, material impact on climate change via CO2 sequestration, and significantly mitigated environmental impacts from energy-related activities and operations.

As part of the Exascale Crosscut, BES will be responsible for the Computational Materials Sciences activities that will support basic research resulting in computer codes to predictively design functional materials, including codes that take full advantage of the future generation of exascale leadership computing capabilities. The report from the foundational workshop for this activity, Computational Materials, Science and Chemistry identified a number of applications that would take full advantage of future computing resources, including: 1) new catalysts to improve the efficiency of industrial processes, make effective use of bioenergy, and drive energy conversion and environment mitigation processes; 2) developing better models of photovoltaic processes and improving the efficiency of photovoltaic devices; and 3) next generation electronic and magnetic materials whose properties are governed by the strong interactions of electrons and have totally new functionalities.

Exascale systems are needed to support areas of research that are critical to national security objectives as well as applied research advances in areas such as climate models, combustion systems, and nuclear reactor design that are not within the capacities of today's systems. Exascale systems' computational power are needed for increasing capable data-analytic and data-intense applications across the entire Federal complex. Exascale is a component of long-term collaboration between the SC's Advanced Scientific Computing Research (ASCR) program and the National Nuclear Security Administration's (NNSA) Advanced Simulation and Computing Campaign (ASC) program.

**FY 2016 Crosscuts (\$K)**

	Subsurface Engineering	Exascale Computing	Total
Basic Energy Sciences	5,000	12,000	17,000

**Basic Energy Sciences  
Funding (\$K)**

	<b>FY 2014 Enacted</b>	<b>FY 2014 Current<sup>1</sup></b>	<b>FY 2015 Enacted</b>	<b>FY 2016 Request</b>	<b>FY 2016 vs. FY 2015</b>
<b>Materials Sciences and Engineering</b>					
Scattering and Instrumentation Sciences Research	64,421	64,421	64,407	67,303	+2,896
Condensed Matter and Materials Physics Research	122,120	122,120	122,120	122,120	0
Materials Discovery, Design, and Synthesis Research	72,424	72,424	72,424	72,424	0
Experimental Program to Stimulate Competitive Research (EPSCoR)	9,953	9,953	9,951	8,520	-1,431
Energy Frontier Research Centers (EFRCs)	50,800	50,800	50,800	55,800	+5,000
Energy Innovation Hubs—Batteries and Energy Storage	24,237	24,237	24,175	24,137	-38
Computational Materials Sciences	0	0	8,000	12,000	+4,000
SBIR/STTR	11,594	0	12,008	12,946	+938
<b>Total, Materials Sciences and Engineering</b>	<b>355,549</b>	<b>343,955</b>	<b>363,885</b>	<b>375,250</b>	<b>+11,365</b>
<b>Chemical Sciences, Geosciences, and Biosciences</b>					
Fundamental Interactions Research	76,794	76,794	76,796	78,726	+1,930
Chemical Transformations Research	93,693	93,693	93,493	93,493	0
Photochemistry and Biochemistry Research	68,599	68,599	68,797	68,797	0
Energy Frontier Research Centers (EFRCs)	49,200	49,200	49,200	54,200	+5,000
Energy Innovation Hubs—Fuels from Sunlight	24,237	24,237	15,000	15,000	0
General Plant Projects (GPP)	600	600	600	600	0
SBIR/STTR	10,093	0	10,350	11,085	+735
<b>Total, Chemical Sciences, Geosciences, and Biosciences</b>	<b>323,216</b>	<b>313,123</b>	<b>314,236</b>	<b>321,901</b>	<b>+7,665</b>
<b>Scientific User Facilities</b>					
Synchrotron Radiation Light Sources	433,050	433,050	447,186	477,079	+29,893
High-Flux Neutron Sources	247,250	247,250	244,113	254,990	+10,877
Nanoscale Science Research Centers (NSRCs)	100,392	100,392	113,649	118,763	+5,114
Other Project Costs	37,400	37,400	9,300	0	-9,300
Major Items of Equipment	45,000	45,000	42,500	35,500	-7,000
Research	40,532	40,532	31,713	34,853	+3,140

<sup>1</sup> Funding reflects the transfer of SBIR/STTR to the Office of Science.

	FY 2014 Enacted	FY 2014 Current <sup>1</sup>	FY 2015 Enacted	FY 2016 Request	FY 2016 vs. FY 2015
SBIR/STTR	27,540	0	27,918	30,664	+2,746
<b>Total, Scientific User Facilities</b>	<b>931,164</b>	<b>903,624</b>	<b>916,379</b>	<b>951,849</b>	<b>+35,470</b>
<b>Subtotal, Basic Energy Sciences</b>	<b>1,609,929</b>	<b>1,560,702</b>	<b>1,594,500</b>	<b>1,649,000</b>	<b>+54,500</b>
<b>Construction</b>					
Linac Coherent Light Source-II (LCLS-II), SLAC	75,700	75,700	138,700	200,300	+61,600
National Synchrotron Light Source-II (NSLS-II), BNL	26,300	26,300	0	0	0
<b>Total, Construction</b>	<b>102,000</b>	<b>102,000</b>	<b>138,700</b>	<b>200,300</b>	<b>+61,600</b>
<b>Total, Basic Energy Sciences</b>	<b>1,711,929</b>	<b>1,662,702</b>	<b>1,733,200</b>	<b>1,849,300</b>	<b>+116,100</b>

SBIR/STTR Funding:

- FY 2014 transferred: SBIR \$43,074,000 and STTR \$6,153,000 (transferred out of BES in FY 2014 Current column)
- FY 2015 projected: SBIR \$44,182,000 and STTR \$6,094,000
- FY 2016 Request: SBIR \$47,561,000 and STTR \$7,134,000

**Basic Energy Sciences**  
**Explanation of Major Changes (\$K)**

<b>FY 2016 vs.  FY 2015</b>
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<p><b>Materials Sciences and Engineering:</b> Additional funds are requested for the Energy Frontier Research Centers to support new centers in strategic areas of material science research that are not represented or are underrepresented in the current EFRC portfolio. The Computational Materials Sciences activity will increase to support additional research that will enable predictive design of functional materials. The Scattering and Instrumentation Sciences Research will increase to support a new investment in midscale instrumentation in the area of ultrafast electron scattering in support of related core research activities.</p>	+11,365
<p><b>Chemical Sciences, Geosciences, and Biosciences:</b> Additional funds are requested for the Energy Frontier Research Centers to support new centers in strategic areas of chemical science, geoscience, and bioscience research that are not represented or are underrepresented in the current EFRC portfolio. The Fuels from Sunlight Energy Innovation Hub is considered for renewal for one final 5-year term starting in September 2015. If the Hub is renewed its scope will be narrowed compared to the first five year period to focus on carbon dioxide reduction. The Fundamental Interactions Research activity will increase to support a new investment in midscale instrumentation in the area of ultrafast electron scattering in support of related core research activities.</p>	+7,665
<p><b>Scientific User Facilities:</b> BES will support near optimal operations of five light sources, including the first full year of operations for the newly constructed National Synchrotron Light Source-II (NSLS-II), five Nanoscale Science Research Centers, and two neutron sources. No funds are requested for the National Synchrotron Light Source. Funding for the Advanced Photon Source Upgrade and NSLS-II Experimental Tools (NEXT) major item of equipment projects will continue per the project plans. FY 2016 is the last year of funding for the NEXT project. No funds are requested for Other Project Costs for the Linac Coherent Light Source-II (LCLS-II) construction project per the project plan.</p>	+35,470
<p><b>Construction:</b> Funding for the LCLS-II construction project will increase per the project plan.</p>	+61,600
<p><b>Total, Basic Energy Sciences</b></p>	<p><b>+116,100</b></p>

## 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.

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

*Advances in fundamental science for superior batteries.* Through the use of sophisticated modeling and experiments, the basic processes that are foundational to the complex systems that comprise batteries are being unraveled to aid in the development of new, superior ways to store energy.

- Atomistic calculations allowed the tailored design of a new binder for lithium-sulfur batteries that resulted in record breaking performance in capacity and lifetime.
- Over 1,500 molecules have been calculated as part of the electrolyte genome with high-throughput, theoretical calculations; these data will be combined with calculations of additional properties, such as their ability to form a solution with metal ions, to select potential high-performance electrolytes for experimental evaluation.
- Analytical characterization of operating batteries demonstrated that the superior charge/discharge rate observed in lithium iron phosphate electrodes is related to the formation of a series of unexpected non-equilibrium compounds during the charge/discharge cycle, opening up the potential composition space for future cathode materials for lithium ion batteries.
- Nanoscale materials continue to provide avenues for improved batteries; highly porous and conductive multi-walled carbon nanotubes were shown to trap polysulfide species and prevent them from forming insoluble compounds, which limit the service life of lithium-sulfur batteries. Trapping the polysulfides would potentially eliminate a major cause for performance degradation.

*Discovery of Novel Porous Materials.* Metal-organic framework (MOF) and related materials are porous structures made up of metal atoms "linked" by rigid organic molecules. Basic research is expanding the potential uses of these versatile materials for gas separations, storage of carbon dioxide and natural gas, and electrical conductors for energy storage applications.

- Using theoretical calculations coupled with characterization with neutron scattering and controlled synthesis, the capture of carbon dioxide was found to increase with chemical tuning and removal of linkers from the molecular MOF framework, providing a new design strategy to optimize carbon dioxide storage and separation.
- MOFs are normally insulators, but by incorporating electrically active organic linkers, MOFs have been designed with electrical conductivities that rival state-of-the-art organic semiconductors currently used in organic photovoltaics. These new porous, conductors have potential uses in novel energy applications such as batteries, supercapacitors, and fuel cells.
- A flexible MOF cage structure was created with a specially designed flexible, organic linker molecule allowing contraction/expansion of the cage by up to 33%. The modified MOF can selectively bind multiple metal ions, a property that could be used for selective recovery of toxic and/or rare earth metal ions and in energy storage applications.

*Fundamental Science Enables Advanced Engine and Fuel Modeling.* Fundamental understanding of chemical reactivity enables validated theories, models and computational tools for predicting rates, products, and dynamics of the chemical processes underlying clean and efficient energy utilization by combustion devices.

- Scientists have produced, observed, and directly measured reaction kinetics of key intermediates (hydroperoxyalkyl radicals) for initiating the combustion process. Such measurements provided deep insights for predictive modeling of the chemistry of autoignition processes in engines.
- Quantum chemical calculations were used for the first time to obtain molecular reaction rates for surrogate biodiesel in combustion reactions. The results revealed that by including tunneling reactions in high-fidelity engine models, predicted engine performance was noticeably impacted. Such calculations significantly improve the fidelity of engine modeling and will assist in the design and optimization of compression-ignition engines.
- Scientists established a new, fundamental theory to predict and model combustion reactions at high pressures and temperatures typical of advanced internal combustion engines. In the new model, mixing is dominated by diffusion of the fuel in a supercritical state, where there is no liquid/gas phase boundary. Experimental evidence at actual operating pressures validates the new theory and further challenges the current classical view of spray atomization in typical diesel engines.

*Atomic-Level Understanding Enables Catalysis by Design.* Fundamental understanding of how atoms bind to surfaces and to molecular targets provides the ability to design ideal catalysts by computer, optimizing reaction efficiency and specificity, before synthesizing them in the laboratory.

- Single palladium atoms were demonstrated for the first time to convert the inert surface of copper into an ultrasensitive catalyst. Binding single metal atoms to a different metal allows for a general strategy to design novel bifunctional heterogeneous catalysts that can be fine-tuned for catalyst selectivity and activity.
- A layered structure of cobalt-molybdenum nitride was discovered to have unexpected catalytic activity and stability similar to that of platinum. The structural knowledge as revealed by x-ray and neutron scattering will aid in the computational search for novel inexpensive compounds with optimal hydrogen electrocatalytic production.
- Using “catalysis by design” principles, scientists predicted novel compositions of nickel-gallium catalysts that experimentally reduce carbon dioxide to methanol at ambient conditions with long-term stability and with higher activity and selectivity than industrial catalysts.

*New devices advance the capabilities at the light source facilities.* Researchers developed improved optics and new detectors to enhance data quality and enable new user experiments.

- At the Stanford Synchrotron Radiation Lightsource, researchers developed a new fabrication method to produce advanced x-ray diffractive nanostructured devices for high resolution, high efficiency manipulation of hard x-rays. At the Advanced Photon Source, scientists developed a new multilayer grating interferometer that was used to

produce high x-ray phase-contrast images. These new optical devices have significantly enhanced the imaging quality at the BES light sources.

- A new tool developed for the Linac Coherent Light Source x-ray laser provides a powerful pulse-by-pulse diagnostic with femtosecond (one quadrillionth of a second) resolution. The new device pinpoints the duration of x-ray pulses to within a few femtoseconds, giving scientists a much more detailed view of the individual pulses that interact with their samples. For the first time scientists can directly measure the x-ray power profile on a shot-by-shot basis with femtosecond resolution, providing a noninvasive diagnostic tool for photon experiments and new insight into lasing dynamics.
- A prototype three-dimensional detector was successfully demonstrated that allowed x-ray data to be taken at the high frame rates needed to explore scientifically challenging problems such as x-ray time-correlation spectroscopy, which require time information on the microsecond scale or better. The breakthrough comprises a two-level microchip that provides twice the area per pixel and allows more on-detector processing than conventional detectors.

*BES user facilities assist industry to advance the frontiers of science and technology.* Researchers from industry use the unique capabilities at the BES scientific user facilities to develop new technologies and new drugs that impact lives.

- Partnering with a leading chip manufacturer, Molecular Foundry researchers developed a new type of extreme ultraviolet photoresist that can be used to manufacture 10 nanometer (nm) node electronic chips, providing a pathway to the next generation technology after the current 14 nm chips. The concept was validated via systematic chemical characterization and could be incorporated into manufacturing lines as early as 2017.
- BES x-ray light source facilities have helped advance the fundamental understanding of how diseases function and how to design drugs to treat them. Recently, scientists used structural information from the Advance Light Source to understand the binding mechanism of a unique antibody that targets multiple cancer types. This led to the development of a unique one-armed antibody that is now in late-stage clinical trials.
- Neutron imaging was used to measure the texture and integrity of internal surfaces of a turbine blade, while parallel residual stress measurements revealed the effects of local heating during the manufacturing process. Collectively, these experiments can help to improve the turbine blade design and enable low cost, energy efficient manufacturing.



## Basic Energy Sciences Materials Sciences and Engineering

### 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 experimental, computational, and tool development research that will 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 and mesoporous 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 science using new tools and techniques to characterize materials structure across multiple length scales and materials dynamics across multiple time scales, and to correlate this data with materials performance under real world conditions.
- **Condensed Matter and Materials Physics**—Understanding the foundations of material functionality and behavior.
- **Materials Discovery, Design, and Synthesis**—Developing the knowledge base and 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 and bio-inspired 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 Energy Frontier Research Centers (EFRCs), the Batteries and Energy Storage Energy Innovation Hub, and Computational Materials Sciences activities. 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. The Computational Materials Sciences activity, initiated in FY 2015, supports integrated, multidisciplinary teams of theorists and experimentalists who focus on development of validated community codes for predictive design of functional materials. This activity will include new approaches to better use the large data sets derived from advanced characterization of materials synthesis, processing, and properties assessments and the parallel data 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. 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 is a growing aspect of this research as is the use of combined scattering techniques to extract heretofore unattainable information on multiple length and time scales.

Recent advances in investigations of materials dynamics are providing a new window into material functions under real world conditions. Ultrafast electron scattering, including diffraction, imaging, and spectroscopy, offers a unique opportunity for understanding structural dynamics and the behavior of matter under conditions far away from equilibrium. Gaining knowledge of the dynamical behavior of materials systems requires characterization tools that can observe structural details in relevant space scales (micron to angstrom) and time scales (femtosecond to microsecond). A new investment in midscale instrumentation funding is requested to support instrumental solutions to enable the development of electron optics and sources, sample environments, and enhanced detectors, to revolutionize our ability to capture and characterize dynamic processes at sub-angstrom spatial resolution and nanosecond temporal resolution. Time-resolved electron probes are complementary to that of x-ray free electron lasers due to the difference in the nature of electron and x-ray scattering. Collectively, these tools provide deeper insight into the dynamic nature of emergent behavior in materials and chemical processes.

### 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. Theoretical research also includes development of computational and data-oriented techniques for materials discovery.

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 design and discovery of new forms of matter with desired 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 design and synthesize 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 and electrocatalysis, solar energy conversion and storage, friction and lubrication, and novel membranes and porous architectures 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, low temperature synthesis approaches of biology to produce semiconductor and magnetic materials under mild 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 in solid state chemistry to enable discovery of new functional materials and the development of new crystal growth methods and thin film deposition techniques to create complex 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 supports research in these states that will develop their scientific capabilities and advance their ability to successfully compete for research funding through open research solicitations. 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 also supports early career researchers in the designated states and territories. EPSCoR is science-driven and supports the most meritorious proposals based on peer review and programmatic priorities.

#### Energy Frontier Research Centers (EFRCs)

The EFRC program, initiated in FY 2009, is a unique 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 that enhance the conversion of electricity to light; the development of the understanding of materials and processes required to enable improved electrical energy storage, efficient separation of gases for carbon capture, and control of defect evolution in radiation environments; and the exploration of phenomena such as superconductivity and spintronics that can optimize energy flow and boost the efficiency of energy transmission. After five years of research activity, the original cohort of 46 EFRCs produced an impressive breadth of accomplishments, including over 5,950 peer-reviewed journal papers, over 275 patent applications and an additional 100 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 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 took place in FY 2014, culminating in the selection of 10 new and 22 renewed EFRCs, based on peer review by external experts. These 32 EFRCs continue to emphasize both grand challenge science and energy use-inspired research. Compared to the original 46 awards, which were 5 year awards, these EFRCs are 4-year awards with funding for the final two years contingent upon successful outcome of a mid-term review. The request for new funding in FY 2016 and the potential recovery of funds from terminations of poorly performing activities after the mid-term review will allow for a new focused EFRC solicitation in FY 2016.

#### 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. As part of their internal evaluation of progress and potential for each research direction to meet the Hub goals, in consultation with BES, JCESR has made shifts in the research thrusts to maximize the impact of resources used in pursuit of these goals. JCESR will also 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. JCESR underwent a management and early operations review in October 2013, and a science-focused review in July 2014. In both cases the review panels provided positive input and recommendations for furthering the JCESR research goals. BES continues to monitor progress closely.

### 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 function and 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 design, discovery, and development of 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. Scientific workshops and National Research Council studies have identified enticing scientific challenges that would advance these goals.<sup>a</sup> 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 requires 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 includes 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. This is also an important topic for U.S. international scientific competitiveness as many of the codes currently used for materials research and engineering were developed outside of the U.S.

To facilitate U.S. leadership in this competitive field, FY 2016 funding will continue support of teams of scientists and engineers who received multi-year awards in FY 2015 to perform the basic research and develop/deliver codes and associated experimental/computational data for the design of functional materials. Additional FY 2016 funding is requested to support research for functional material topics not supported in FY 2015. Each research team will focus on a different area of functional materials. BES management and coordination among the teams would further leverage activities and accelerate key foundational research. An ideal end product for this research is 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

<sup>a</sup> 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.

annual peer reviews to assess progress towards planned scientific goals. Early in the award period, each funded research team will be reviewed, with a focus on management and early research activities.

**Basic Energy Sciences  
Materials Sciences and Engineering**

**Activities and Explanation of Changes**

FY 2015 Enacted	FY 2016 Request	Explanation of Changes FY 2016 vs. FY 2015
<b>Materials Sciences and Engineering \$363,885,000</b>	<b>\$375,250,000</b>	<b>+\$11,365,000</b>
<b>Scattering and Instrumentation Sciences Research (\$64,407,000)</b>	<b>(\$67,303,000)</b>	<b>(+\$2,896,000)</b>
<p>Time domain, energy spectroscopy, and <i>in situ</i> 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 is 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.</p>	<p>Ultrafast science will continue to be a priority research area. Mid-scale instrumentation will support development of electron optics and sources, sample environments, and enhanced detectors to revolutionize our ability to capture and characterize dynamic processes at sub-angstrom spatial resolution and nanosecond temporal resolution. For x-rays, vacuum ultraviolet, and other lower frequency sources however, future investments will emphasize hypothesis-driven research with existing ultrafast science capabilities to establish a more complete understanding of materials properties and behaviors. Neutron scattering sciences will stress innovative time-of-flight scattering and imaging and their effective use in transformational research. New advances in spectroscopy, high-resolution analyses of energy-relevant soft matter, and quantitative <i>in situ</i> analysis capabilities under perturbing parameters such as temperature, stress, chemical environment, and magnetic and electric fields will be pursued.</p>	<p>Increased funding will be used to support mid-scale instrumentation related to ultrafast electron diffraction. For the balance of the research program, areas of increased emphasis involve hypothesis-driven ultrafast science and time-resolved imaging and energy excitation spectroscopy with high spatial resolution. A strong focus will be directed towards understanding scientific phenomena on real systems under realistic operating conditions. Research with traditional microscopy and x-ray techniques will be deemphasized.</p>

FY 2015 Enacted	FY 2016 Request	Explanation of Changes FY 2016 vs. FY 2015
<b>Condensed Matter and Materials Physics Research (\$122,120,000)</b>	<b>(\$122,120,000)</b>	<b>(\$0)</b>
<p>Research continues to support experimental and theoretical materials research emphasizing correlation effects, including phenomena observed in topological surface states. The program emphasizes 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 continues 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 continues to grow research on new theoretical tools and validated software for materials discovery. The research continues to advance fundamental understanding of defects to extend the lifetime and enhance performance of materials in energy generation and energy end-use applications.</p>	<p>The program will continue to support fundamental experimental and theoretical research on the properties of materials. It will focus on structural, optical, and electrical properties and control of material functionality in response to external stimuli including temperature, pressure, magnetic and electric fields, and radiation. Phenomena in materials will be investigated from atomistic through nanoscale to mesoscale length scales. The research supported will continue to address defect structures in materials and how these influence materials properties, especially in energy relevant materials. There is an ongoing emphasis on understanding the relationship between electronic structure and properties in materials that exhibit correlation effects. Research on spin physics, focusing on coupling across heterogeneous boundaries through spin orbit and exchange interactions and studies involving novel magneto-dynamics, will be continued. Research involving theory and computational data coupled to experimental characterization of material properties will continue to grow.</p>	<p>Research support is level compared to FY 2015. The FY 2016 program will enhance research understanding of matter at atomistic length scales expanding to include properties at the mesoscale. Research on granular materials, conventional superconductivity, high strain rate, high dose radiation effects, and cold atom physics will be de-emphasized.</p>



FY 2015 Enacted	FY 2016 Request	Explanation of Changes FY 2016 vs. FY 2015
<b>Materials Discovery, Design, and Synthesis Research (\$72,424,000)</b>	<b>(\$72,424,000)</b>	<b>(\$0)</b>
<p>Research continues 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 <i>in situ</i> 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.</p>	<p>Research on the predictive design and synthesis of materials across multiple length scales will continue with a particular emphasis on the mesoscale, where functionalities begin to emerge. Within this framework, a fundamental understanding of assembly, both self and directed, and interfacial phenomena, ubiquitous in all materials, will be developed. Additionally, synthesis pathways will be better understood by use of <i>in situ</i> diagnostics and characterization so that they can be controlled more precisely and dynamically. This research will help realize the visionary goals of atom- and energy-efficient syntheses of new forms of matter. Research on recent energy materials on the scene, such as perovskite photovoltaic materials and those with 2D topologies, will be strengthened to take advantage of the opportunities to realize a more thorough understanding and their potential for bringing about transformational advances in energy and information technologies.</p>	<p>Research support is level compared to FY 2015. The program will explore a new direction-dissipative assembly of active matter, i.e., material systems capable of transducing, storing and/or harvesting energy, emulating those found in nature. This will entail experimental materials synthesis research to be integrated even more closely with computational tools and resources. Research on developing synthesis methods for nanomaterials, e.g., nanoparticles, nanorods, etc. will be deemphasized.</p>
<b>Experimental Program to Stimulate Competitive Research (EPSCoR) (\$9,951,000)</b>	<b>(\$8,520,000)</b>	<b>(-\$1,431,000)</b>
<p>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 are sustained.</p>	<p>Efforts will continue to span science in support of the DOE mission, with continued emphasis on science that underpins DOE energy technology programs. Implementation grant, state-laboratory partnerships, and investment in early career research staff from EPSCoR states will be sustained.</p>	<p>The request is lower than the FY 2015 appropriation. The additional funding provided in FY 2015 is being used to minimize outyear mortgages for implementation grants.</p>

FY 2015 Enacted	FY 2016 Request	Explanation of Changes FY 2016 vs. FY 2015
<b>Energy Frontier Research Centers (EFRCs) (\$50,800,000)</b>	<b>(\$55,800,000)</b>	<b>(+\$5,000,000)</b>
<p>The EFRCs that were started in FY 2014 are performing the first year of research of the award period as outlined in their proposals. This multidisciplinary research continues 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.</p>	<p>The EFRCs will continue to perform fundamental multi-disciplinary research aimed at accelerating scientific innovation. All EFRCs will undergo a mid-term review in FY 2016 to assess progress toward meeting scientific research goals. DOE will issue a Funding Opportunity Announcement for up to five new EFRC awards in FY 2016.</p>	<p>The total BES EFRC program is increased by \$10,000,000 compared to FY 2015, which is split equally between Materials Sciences and Engineering and Chemical Sciences, Geosciences, and Biosciences. New EFRCs funded through this subprogram will focus on strategic areas of material science research that are not represented or are underrepresented in the current EFRC portfolio.</p>
<b>Energy Innovation Hubs—Batteries and Energy Storage (\$24,175,000)</b>	<b>(\$24,137,000)</b>	<b>(-\$38,000)</b>
<p>Research continues 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 include techno-economic modeling, cell design, and preliminary prototype development. Research includes a focus on the electrolyte genome, demonstrating the utility of this computational framework for designing new electrolytes using structure-chemical trends extracted from &gt;10,000 first-principles calculated molecular motifs, modifications and mutations.</p>	<p>The Hub, in its fourth year, will continue to follow its project plan with an increasing focus on developing lab-scale prototypes to supplement the ongoing fundamental research science underpinning batteries for transportation and the grid, as well as cross-cutting research on materials characterization, theory, and modeling. JCESR will complete self-consistent system analyses using techno-economic modeling of three electrochemical couples identified through materials discovery, including output from the electrolyte genome, that have the potential to meet technical performance and cost criteria.</p>	<p>The funding is approximately level compared to FY 2015, following the planned funding profile.</p>

FY 2015 Enacted	FY 2016 Request	Explanation of Changes FY 2016 vs. FY 2015
<b>Computational Materials Sciences (\$8,000,000)</b>	<b>(\$12,000,000)</b>	<b>(+\$4,000,000)</b>
<p>Coupling today’s computational capabilities with world leading experimental instrumentation, the Computational Materials Sciences activity enhances 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 supports 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 supports the first year of multi-year awards.</p>	<p>Computational Materials Sciences will advance U.S. leadership in the development of computational codes for materials sciences and engineering. The research activities involve teams of theorists, computational experts, and experimentalists with expertise in synthesis, characterization, and processing/fabrication of materials. The computational materials sciences teams that will start in FY 2015 will perform the first year of research as outlined in their proposals. This research will focus on basic science necessary to develop research-oriented, open-source, experimentally validated software and the associated databases required to predictively design materials with specific functionality. Funding will support additional multi-year awards for research teams focused on functional materials topics not supported by the FY 2015 awards. Early in the award period, each team will be peer reviewed to assess management and early research activities.</p>	<p>In addition to supporting the ongoing research for the FY 2015 awards, the FY 2016 request will broaden the technical breadth of the research to include new awards to teams focused on additional types of materials functionality.</p>



## Basic Energy Sciences Chemical Sciences, Geosciences, and Biosciences

### 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, photo electrochemistry, 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. This activity also 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. The FY 2016 request includes support for a new investment in midscale instrumentation to support development of ultrafast electron scattering probes. This activity will focus on achieving time-resolved mapping of structural molecular changes during chemical reactions. In time-resolved electron diffraction, very short electron pulses are applied to monitor chemical transformations in real time. The technique has been demonstrated for simple reactions in the condensed phase, but the challenge is even greater for reactions in the gas phase. Developments are underway that allow the pinning of gas molecules using laser pulses but have only been demonstrated for simple molecules. The development of innovative instrumentation for ultrafast electron scattering will help address these challenges. Time-resolved electron probes are complementary to that of x-ray free electron lasers due to the difference in the nature of electron and x-ray scattering. Collectively, these tools provide deeper insight into the dynamic nature of emergent behavior in materials and chemical processes.

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, the chemistry of actinides important to 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.

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 used 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 (EFRCs)

The EFRC program, initiated in FY 2009, is a unique 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 following topics: 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; and for science-based carbon capture and geological sequestration. After five years of research activity, the original cohort of 46 EFRCs produced an impressive breadth of accomplishments, including over 5,950 peer-reviewed journal papers, over 275 patent applications, and an additional 100 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 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.

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#### 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*,<sup>a</sup> 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, called 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 received the final year of funding for its initial five-year award term at the planned level in FY 2014. As part of BES oversight of this Hub, JCAP has been evaluated via peer review on an annual basis since the initiation of the project. Following the latest scientific and technical review conducted in April 2014, BES determined that JCAP was on target to satisfy both its five-year goal as originally proposed and the performance milestones set forth as renewal criteria in the 2012 Energy Innovation Hubs Report to Congress. Given the latest review results, JCAP's overall scientific and technological progress, and the distinct role of this Hub in the BES research portfolio, JCAP is being considered for a final term of renewal with a maximum duration of five years. A renewal would allow JCAP to capitalize on its achievements during the initial funding period and to further advance research efforts addressing critical needs in solar fuels development. The Department will make a renewal determination based on the outcome of an external peer review. If the Department recommends renewal, JCAP will be directed to initiate a restructured research and development plan focused primarily on discovery science for efficient solar-driven production of carbon-based fuels. The reduced funding level for a potential renewal award term compared to the first award term reflects a de-emphasized research scope both on water oxidation and on design and development of prototypes. This renewal plan is consistent with options suggested in the 2014 report from the Secretary of Energy Advisory Board, *Task Force Report to Support the Evaluation of New Funding Constructs for Energy R&D in the DOE*.

<sup>a</sup> U.S. DOE Basic Energy Sciences Advisory Committee. *New Science for a Secure and Sustainable Energy Future*. U.S. Department of Energy Office of Science, 2008.



### 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.

**Basic Energy Sciences  
Chemical Sciences, Geosciences, and Biosciences**

**Activities and Explanation of Changes**

FY 2015 Enacted	FY 2016 Request	Explanation of Changes FY 2016 vs. FY 2015
<b>Chemical Sciences, Geosciences, and Biosciences \$314,236,000</b>	<b>\$321,901,000</b>	<b>+\$7,665,000</b>
<b>Fundamental Interactions Research (\$76,796,000)</b>	<b>(\$78,726,000)</b>	<b>(+\$1,930,000)</b>
<p>Research continues 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 are sought to guide and interpret ultrafast measurements and for predicting ultrafast phenomena. Increased emphasis is placed on time-resolved x-ray probes of matter at unprecedented short time scales and in systems of substantial complexity. These 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 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 continues on advanced combustion research to accelerate the predictive simulation of highly efficient and clean internal combustion engines. Increased emphasis is placed on investigating properties of combustion in high-pressure or multiphase systems.</p>	<p>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, to probe and control atomic, molecular, nanoscale and mesoscale matter. New efforts in mid-scale instrumentation will support development of electron scattering techniques that enable the probing of intermediate molecular states in chemical reaction dynamics. The current limitation in gas phase experiments is the velocity mismatch in timescale between electron and laser pulses that limit such investigations to the picosecond timescale. Advanced theoretical methods will be developed to guide and interpret ultrafast measurements and to design new experiments. Emphasis will continue to be placed on time-resolved electron and x-ray probes of matter at unprecedented short time scales and in systems of increasing complexity. Computational efforts will stress the development of improved methods to calculate electronically excited states in molecules and extended mesoscale systems. Work will continue on advanced combustion research to accelerate the predictive simulation of highly efficient and clean internal combustion engines. Increased emphasis will be on investigating properties of combustion in high-</p>	<p>Research support increases compared to FY 2015 for investments in mid-scale instrumentation for chemical imaging at the limits of temporal and spatial resolution. Emphasis will be placed on diffraction induced by femtosecond electron pulses that reveals time resolved dynamics of chemical processes. 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 ultrafast phenomena will be enhanced, and research on ultra cold molecules will be deemphasized. Well-developed research topics in molecular and particle spectroscopy may be redirected to evolving forefront areas, such as energy transfer in molecular systems, and the effects of solvation and interfaces on chemical structure and reactivity.</p>

FY 2015 Enacted	FY 2016 Request	Explanation of Changes FY 2016 vs. FY 2015
pressure or multiphase systems.		
<b>Chemical Transformations Research (\$93,493,000)</b>	<b>(\$93,493,000)</b>	<b>(\$0)</b>
<p>Research continues 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 is 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 continue with added integration with computational methods. Research continues 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 continues, 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 support new efforts in carbon capture and sequestration as well as research in geophysical characterization and monitoring techniques.</p>	<p>Synthesis, guided by theory and computation, will continue to explore novel catalytic materials at the nano- and mesoscale for the efficient conversion of traditional and new feedstocks into higher-value fuels and other chemicals. The catalytic conversion of biomass to fuels and other energy related chemical products will be emphasized. Likewise, coupled predictive theory and synthesis of designer mesoporous membranes and filter materials will seek more efficient separation of carbon dioxide from conventional power plant effluents or of oxygen from air relevant to oxycombustion approaches. Subsurface geochemistry and geophysics will seek to provide data and mechanistic interpretation for models of reactive flow and transport important for carbon sequestration and extraction of tight gas and oil. Actinide research will continue to emphasize new insights in actinides chemical bonding enabling new chemistry for separation and related nuclear fuels and waste form processes especially using ionic liquids. Fundamental research activities in geochemistry and geophysics of the subsurface will continue in FY 2016 in parallel with efforts in other offices as coordinated by the Subsurface Technology and Engineering RD&amp;D (SubTER) technology integration team.</p>	<p>Research support is level compared to FY 2015. Areas of increased emphasis include integration of computational and theoretical modeling methods with energy-relevant catalytic chemistries and subsurface imaging. Some mature areas of research in polymer synthesis, liquid-liquid extraction techniques, and surface geophysics may be decreased.</p>

FY 2015 Enacted	FY 2016 Request	Explanation of Changes FY 2016 vs. FY 2015
<b>Photochemistry and Biochemistry Research (\$68,797,000)</b>	<b>(\$68,797,000)</b>	<b>(\$0)</b>
<p>Research on fundamental aspects of light energy capture and conversion in non-biological and biological (photosynthetic) systems continues 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 enables 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, provides 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 helps inform catalytic strategies for the direct conversion of biomass to fuels and other products.</p>	<p>Research will continue to emphasize a fundamental understanding of light energy capture and conversion in non-biological and biological (photosynthetic) systems. These studies will establish a foundation for direct conversion of solar energy to electricity, fuels, and high value chemicals. Efforts in computation and modeling will continue to be supported as such approaches can facilitate design and fabrication of semiconductor/polymer interfaces, dye-sensitized solar cells, inorganic-organic molecular complexes, and bio-inspired/biohybrid light harvesting complexes. Research to understand the fundamental mechanisms of water-splitting, redox, cell wall biosynthesis, and other energy-relevant biological (enzymatic) reactions, from the nano- to the mesoscale, will continue to be emphasized. These studies will provide new insights for developing novel bio-inspired catalysts based on earth-abundant materials and for controlling and optimizing chemical reactions important for energy capture, conversion, and storage.</p>	<p>Research support is level compared to FY 2015. Efforts in the study of plant hormones, biotic stress and on the development of genetic systems will be de-emphasized. Greater emphasis will be placed on understanding the structure, function, and mechanism of enzymes that mediate the flow of electrons in biological systems.</p>

FY 2015 Enacted	FY 2016 Request	Explanation of Changes FY 2016 vs. FY 2015
<b>Energy Frontier Research Centers (EFRCs)</b> <b>(\$49,200,000)</b>	<b>(\$54,200,000)</b>	<b>(+\$5,000,000)</b>
<p>The EFRCs that were started in FY 2014 are performing the first year of research of the award period as outlined in their proposals. This multidisciplinary research continues 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.</p>	<p>The EFRCs will continue to perform fundamental multi-disciplinary research aimed at accelerating scientific innovation. All EFRCs will undergo a mid-term review in FY 2016 to assess progress toward meeting scientific research goals. DOE will issue a Funding Opportunity Announcement for up to five new EFRC awards in FY 2016.</p>	<p>The total BES EFRC program is increased by \$10,000,000 compared to FY 2015, which is split equally between Materials Sciences and Engineering and Chemical Sciences, Geosciences, and Biosciences. New EFRCs funded through this subprogram will focus on strategic areas of chemical science, geoscience, and bioscience that are not represented or are underrepresented in the current EFRC portfolio.</p>
<b>Energy Innovation Hubs—Fuels From Sunlight</b> <b>(\$15,000,000)</b>	<b>(\$15,000,000)</b>	<b>(\$0)</b>
<p>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 January 2015.</p>	<p>The Fuels from Sunlight Hub will be considered for the final term of renewal for up to 5 years starting in September 2015. The renewal would allow JCAP to capitalize on its achievements during the initial funding period and to further advance research efforts addressing critical needs in solar fuels development. The Department will base its renewal decision on the outcome of an external peer review.</p>	<p>If a renewal is awarded, the research scope of the renewal project will build on the accomplishments of the first phase of the JCAP award in hydrogen production and expand to CO<sub>2</sub> reduction for carbon-based fuel formation. JCAP will support a restructured research and development plan focused primarily on discovery science for efficient solar-driven production of carbon-based fuels. The reduced funding level compared to the first award term reflects a de-emphasized research scope on water oxidation and on design and development of prototypes.</p>
<b>General Plant Projects (\$600,000)</b>	<b>(\$600,000)</b>	<b>(\$0)</b>
<p>Funding supports minor facility improvements at Ames Laboratory.</p>	<p>Funding will support minor facility improvements at Ames Laboratory.</p>	<p>General Plant Projects is level compared to FY 2015.</p>



## Basic Energy Sciences Scientific User Facilities

### Description

The Scientific User Facilities subprogram supports the operation of a geographically diverse suite of major research 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 newly constructed National Synchrotron Light Source-II (NSLS-II) at Brookhaven National Laboratory (BNL). 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.

#### High Flux Neutron Sources

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, thermal 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 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 19 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. The final three instruments were completed in 2014 from the SNS Instrumentation Next Generation-II (SING-II) major item of equipment project: the ultra-small angle diffractometer, the elastic diffuse scattering spectrometer, and the macromolecular neutron diffractometer. All the SNS instruments are in high demand by researchers world-wide in a range of disciplines from biology to materials sciences and condensed matter physics.

#### Nanoscale Science Research Centers (NSRCs)

Nanoscience is the study of materials and their behaviors at the nanometer scale—probing and assembling single atoms, clusters of atoms, and molecular structures. The scientific quest is to design new nanoscale materials and structures, and observe and understand how they function, including how they interact with their environment. Developments at the



nanoscale and mesoscale 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 and assembly 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 atomic-scale 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 with a total project cost greater than \$5,000,000 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 and developing ultrafast electron diffraction systems that complement the

capabilities of x-ray FELs. This activity also includes research in sophisticated data management tools to address the vastly accelerated pace and volume of data generated by faster, higher resolution detectors and brighter light sources.

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 is merged administratively with its respective neighboring NSRCs.

**Basic Energy Sciences  
Scientific User Facilities**

**Activities and Explanation of Changes**

FY 2015 Enacted	FY 2016 Request	Explanation of Changes FY 2016 vs. FY 2015
<b>Scientific User Facilities \$916,379,000</b>	<b>\$951,849,000</b>	<b>+\$35,470,000</b>
<b>Synchrotron Radiation Light Sources (\$447,186,000)</b>	<b>(\$477, 079,000)</b>	<b>(+\$29,893,000)</b>
The FY 2015 appropriation supports operations of the BES light source facilities, including early operations for the newly constructed NSLS-II, at below optimal levels. NSLS ceases operations and transitions to a safe storage condition in FY 2015.	In FY 2016, funding is requested for near optimal operations of the five BES light sources, including the first full year of operations for the newly constructed NSLS-II. No funding is requested for NSLS.	The funding increase will support operations at near optimal levels for the light sources. It will allow the facilities to proceed with the most critical deferred repairs and replacements of outdated instruments, essential accelerator improvements, and limited staff hires or replacements. The request will also support the increased cost of power and user support.
<b>High-Flux Neutron Sources (\$244,113,000)</b>	<b>(\$254,990,000)</b>	<b>(+\$10,877,000)</b>
Funding is provided to continue the operation of HFIR and SNS at below optimal levels. BES operations at the Lujan Neutron Scattering Center cease and the facility transitions to a safe storage condition.	Funding is requested to continue the operation of HFIR and SNS at near optimal levels. Limited funding is requested for the Lujan Neutron Scattering Center for the removal of hazardous materials and planning of the disposition of unused equipment.	The funding increase will support operations at near optimal levels for HFIR and SNS. It will allow the facilities to proceed with the most critical deferred repairs and replacements of outdated instruments, essential machine improvements, and limited staff hires or replacements. The request will also support the increased cost of power and user support.

FY 2015 Enacted	FY 2016 Request	Explanation of Changes FY 2016 vs. FY 2015
<b>Nanoscale Science Research Centers (\$113,649,000)</b>	<b>(\$118,763,000)</b>	<b>(+\$5,114,000)</b>
Funding supports continuing operations and support of users at the NSRCs at below optimal level. The electron-beam microcharacterization centers (EBMCs) merge with the NSRCs in FY 2015. Continued program emphasis cultivates and expands the user base from universities, national laboratories, and industry. Efforts include planning for future electron scattering needs that address scientific roadblocks toward observing ultrafast chemical and physical phenomena at ultra-small size scales in different sample environments.	Funding is requested to continue operations and support of users at the NSRCs at near optimal levels. Program emphasis will continue to cultivate and expand the user base from universities, national laboratories, and industry. Planning efforts will continue to advance the cutting-edge nanostructure characterization capabilities, with an emphasis on coupling multi-probes of photon, neutron, and electron, and 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.	The funding increase will support operations at near optimal levels for the NSRCs.
<b>Other Project Costs (\$9,300,000)</b>	<b>(\$0)</b>	<b>(-\$9,300,000)</b>
Funds for Other Project Costs are associated with the LCLS-II project at SLAC and follow the project plan.	No funds are requested for Other Project Costs in FY 2016.	Other Project Costs decreases according to the LCLS-II project plan.
<b>Major Items of Equipment (\$42,500,000)</b>	<b>(\$35,500,000)</b>	<b>(-\$7,000,000)</b>
APS-U continues with planning and design, magnet prototyping, and research and development related to implementation of the multi-bend achromat lattice during FY 2015.	APS-U will continue with planning and facility design, magnet prototyping, and research and development related to implementation of the multi-bend achromat lattice during FY 2016.	APS-U funding is level with FY 2015.
NEXT continues with the design, procurements, construction/fabrication, installation, testing and commissioning of equipment during FY 2015.	NEXT will continue with the design, procurements, construction/fabrication, installation, testing and commissioning of equipment during FY 2016.	NEXT funding decreases according to the project profile. FY 2016 is the final year of funding for this project.

FY 2015 Enacted	FY 2016 Request	Explanation of Changes FY 2016 vs. FY 2015
<b>Research (\$31,713,000)</b>	<b>(\$34,853,000)</b>	<b>(+\$3,140,000)</b>
<p>The research funding for the scientific user facilities supports efforts in x-ray optics developments and data management techniques, and continues 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) merges 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.</p>	<p>The research funding for the scientific user facilities will continue to support selected, high-priority research activities. This funding will support activities to ensure that the scientific user facilities continue to demonstrate performance excellence, with focused efforts to address next generation facilities research needs. Emphasis will also be placed on detectors and optics instrumentation to allow full utilization of neutron and photon beams. Funding to continue the long term surveillance and maintenance responsibilities at BNL and SLAC is also included in this portion of the budget.</p>	<p>The increase in funding will allow expansion of research activities addressing new accelerator needs, detector and optics instrumentation, and the growing demands for data management tools by a wide spectrum of users.</p>



## **Basic Energy Sciences Construction**

### **Description**

Reactor-based neutron sources, accelerator-based x-ray light sources, and accelerator-based pulsed neutron sources are essential 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.

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 was 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.

**Basic Energy Sciences  
Construction**

**Activities and Explanation of Changes**

FY 2015 Enacted	FY 2016 Request	Explanation of Changes FY 2016 vs. FY 2015
<b>Construction \$138,700,000</b>	<b>\$200,300,000</b>	<b>+\$61,600,000</b>
<b>Linac Coherent Light Source-II (LCLS-II) (\$138,700,000)</b>	<b>(\$200,300,000)</b>	<b>(+\$61,600,000)</b>
The project continues with facility design, initiates critical long-lead procurements of technical materials and cryogenic systems, continues research and development and prototyping activities, and fabrication of technical equipment during FY 2015.	The project will complete facility design, and continue research and development, prototyping, construction, and fabrication and installation of technical equipment during FY 2016.	LCLS-II funding is increased according to the project profile. The increased funding supports continuation of construction and installation activities.



**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.

	FY 2014	FY 2015	FY 2016
Performance Goal (Measure)	<b>BES Facility Operations—Average achieved operation time of BES user facilities as a percentage of total scheduled annual operation time</b>		
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)	<b>BES Facility Construction/MIE Cost &amp; Schedule—Cost-weighted mean percent variance from established cost and schedule baselines for major construction, upgrade, or equipment procurement projects.</b>		
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.		
Performance Goal (Measure)	<b>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</b>		
Target	Design first prototype device for testing components, such as catalysts, light harvesters, membranes, and interfaces, as an integrated system	N/A	N/A
Result	Met	N/A	N/A
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 <i>Fuels from Sunlight</i> Energy Innovation Hub.		

	FY 2014	FY 2015	FY 2016
Performance Goal (Measure)	<b>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.</b>		
Target	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.	Complete self-consistent system analyses using techno-economic modeling of three electrochemical couples, identified through materials discovery including output from the electrolyte genome, that have the potential to meet technical performance and cost criteria.
Result	N/A	TBD	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 <i>Batteries and Energy Storage</i> Energy Innovation Hub.		

**Basic Energy Science  
Capital Summary (\$K)**

	<b>Total</b>	<b>Prior Years</b>	<b>FY 2014 Enacted</b>	<b>FY 2014 Current</b>	<b>FY 2015 Enacted</b>	<b>FY 2016 Request</b>	<b>FY 2016 vs. FY 2015</b>
<b>Capital Operating Expenses Summary</b>							
Capital Equipment	n/a	n/a	63,068	63,068	48,100	41,000	-7,100
General Plant Projects (GPP)	n/a	n/a	600	600	600	600	0
Accelerator Improvement Projects (AIP)	n/a	n/a	13,000	13,000	9,925	9,425	-500
<b>Total, Capital Operating Expenses</b>	<b>n/a</b>	<b>n/a</b>	<b>76,668</b>	<b>76,668</b>	<b>58,625</b>	<b>51,025</b>	<b>-7,600</b>
<b>Capital Equipment</b>							
Major Items of Equipment							
Advanced Photon Source Upgrade (APS-U), ANL (TPC TBD) <sup>a</sup>	TBD	40,000	20,000	20,000	20,000	20,000	0
Linac Coherent Light Source-II (LCLS-II), SLAC <sup>b,c</sup>	—	67,000	0	0	0	0	0
NSLS-II Experimental Tools (NEXT), BNL (TPC \$90,000)	90,000	27,000	25,000	25,000	22,500	15,500	-7,000
Total, Major Items of Equipment	n/a	n/a	45,000	45,000	42,500	35,500	-7,000
Other capital equipment projects under \$2 million TEC	n/a	n/a	18,068	18,068	5,600	5,500	-100
<b>Total, Capital equipment</b>	<b>n/a</b>	<b>n/a</b>	<b>63,068</b>	<b>63,068</b>	<b>48,100</b>	<b>41,000</b>	<b>-7,100</b>
<b>General Plant Projects (GPP)</b>							
Other general plant projects under \$5 million TEC	n/a	n/a	600	600	600	600	0
<b>Total, General Plant Projects</b>	<b>n/a</b>	<b>n/a</b>	<b>600</b>	<b>600</b>	<b>600</b>	<b>600</b>	<b>0</b>
<b>Accelerator Improvement Projects (AIP)</b>							
Accelerator improvement projects under \$5 million TEC	n/a	n/a	13,000	13,000	9,925	9,425	-500

<sup>a</sup> Following the July 2013 BESAC report on Future X-Ray Light Sources, the APS-U project has been rescoped and a revised Mission Need Statement is in preparation.

<sup>b</sup> LCLS-II is requested as a line item construction project beginning in FY 2014.

<sup>c</sup> LCLS-II received \$85,600,000 in FY 2010-FY 2013 as an MIE.

## **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 under load conditions. All three foreign facilities are well into campaigns of major upgrades of beamlines and are also incorporating technological advancements in accelerator science to enhance performance. 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. x-ray arsenal that are a pre-requisite for tackling the grand science and energy challenges of the 21<sup>st</sup> 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 100-1000 times increased brightness. 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 x-ray free electron lasers (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)**

	<b>Total</b>	<b>Prior Years</b>	<b>FY 2014 Enacted</b>	<b>FY 2014 Current</b>	<b>FY 2015 Enacted</b>	<b>FY 2016 Request</b>	<b>FY 2016 vs. FY 2015</b>
<b>13-SC-10, Linac Coherent Light Source-II (LCLS-II), SLAC</b>							
TEC	916,400	67,000	75,700	75,700	138,700	200,300	+61,600
OPC	48,600	18,600	10,000	10,000	9,300	0	-9,300
<b>TPC</b>	<b>965,000</b>	<b>85,600<sup>a</sup></b>	<b>85,700</b>	<b>85,700</b>	<b>148,000</b>	<b>200,300</b>	<b>+52,300</b>
<b>07-SC-06, National Synchrotron Light Source-II, BNL</b>							
TEC	791,200	764,900	26,300	26,300	0	0	+/-0,000
OPC	120,800	93,400	27,400	27,400	0	0	+/-0,000
<b>TPC</b>	<b>912,000</b>	<b>858,300</b>	<b>53,700</b>	<b>53,700</b>	<b>0</b>	<b>0</b>	<b>+/-0,000</b>
<b>Total, Construction</b>							
TEC	n/a	n/a	102,000	102,000	138,700	200,300	+61,600
OPC	n/a	n/a	37,400	37,400	9,300	0	-9,300
<b>TPC</b>	<b>n/a</b>	<b>n/a</b>	<b>139,400</b>	<b>139,400</b>	<b>148,000</b>	<b>200,300</b>	<b>+52,300</b>

**Funding Summary (\$K)**

	<b>FY 2014 Enacted</b>	<b>FY 2014 Current</b>	<b>FY 2015 Enacted</b>	<b>FY 2016 Request</b>	<b>FY 2016 vs. FY 2015</b>
Research	697,010	697,010	686,876	707,373	+20,497
Scientific User Facilities Operations	780,692	780,692	804,948	850,832	+45,884
Major Items of Equipment	45,000	45,000	42,500	35,500	-7,000
Construction Projects (includes OPC)	139,400	139,400	148,000	200,300	+52,300
Other <sup>b</sup>	49,827	600	50,876	55,295	+4,419
<b>Total, Basic Energy Sciences</b>	<b>1,711,929</b>	<b>1,662,702</b>	<b>1,733,200</b>	<b>1,849,300</b>	<b>+116,100</b>

<sup>a</sup> LCLS-II received \$85,600,000 in FY 2010-FY 2013 as an MIE.

<sup>b</sup> Includes SBIR/STTR funding and non-Facility related GPP.

### Facility Operations (\$K)

The treatment of user facilities is distinguished between two types: TYPE A facilities that offer users resources dependent on a single, large-scale machine; TYPE B facilities that offer users a suite of resources that is not dependent on a single, large-scale machine.

**Definitions:**

Achieved Operating Hours – The amount of time (in hours) the facility was available for users.

Planned Operating Hours –

- For Past Fiscal Year (PY), the amount of time (in hours) the facility was planned to be available for users.
- For Current Fiscal Year (CY), the amount of time (in hours) the facility is planned to be available for users.
- For the Budget Fiscal Year (BY), based on the proposed budget request the amount of time (in hours) the facility is anticipated to be available for users.

Optimal Hours – The amount of time (in hours) a facility would be available to satisfy the needs of the user community if unconstrained by funding levels.

Percent of Optimal Hours – An indication of utilization effectiveness in the context of available funding; it is not a direct indication of scientific or facility productivity.

- For BY and CY, Planned Operating Hours divided by Optimal Hours expressed as a percentage.
- For PY, Achieved Operating Hours divided by Optimal Hours.

Unscheduled Downtime Hours - The amount of time (in hours) the facility was unavailable to users due to unscheduled events. NOTE: For type “A” facilities, zero Unscheduled Downtime Hours indicates Achieved Operating Hours equals Planned Operating Hours.

	FY 2014 Enacted	FY 2014 Current	FY 2015 Enacted	FY 2016 Request	FY 2016 vs. FY 2015
<b>TYPE A FACILITIES</b>					
<b>Advanced Light Source</b>	<b>\$60,000</b>	<b>\$60,000</b>	<b>\$60,500</b>	<b>\$63,223</b>	<b>+2,723</b>
Number of Users	2,443	2,443	2,400	2,450	+50
Achieved operating hours	4,838	4,838	N/A	N/A	
Planned operating hours	5,100	5,100	5,000	5,200	+200
Optimal hours	5,300	5,300	5,300	5,300	0
Percent optimal hours	91.3%	91.3%	94.3%	98.1%	
Unscheduled downtime hours	<10%	<10%	<10%	<10%	

	FY 2014 Enacted	FY 2014 Current	FY 2015 Enacted	FY 2016 Request	FY 2016 vs. FY 2015
<b>Advanced Photon Source</b>	<b>\$122,800</b>	<b>\$122,800</b>	<b>\$124,815</b>	<b>\$130,432</b>	<b>+5,617</b>
Number of Users	5,017	5,017	5,000	5,100	+100
Achieved operating hours	4,901	4,901	N/A	N/A	
Planned operating hours	5,000	5,000	5,000	5,000	0
Optimal hours	5,000	5,000	5,000	5,000	0
Percent optimal hours	98.0%	98.0%	100%	100%	
Unscheduled downtime hours	<10%	<10%	<10%	<10%	
<b>National Synchrotron Light Source, BNL</b>	<b>\$29,900</b>	<b>\$29,900</b>	<b>\$5,500</b>	<b>\$0</b>	<b>-5,500</b>
Number of Users	2,372	2,372	0	0	0
Achieved operating hours	5,848	5,848	N/A	N/A	
Planned operating hours	4,400	4,400	0	0	0
Optimal hours	4,500	4,500	0	0	0
Percent optimal hours	130.0%	130.0%	N/A	N/A	
Unscheduled downtime hours	<10%	<10%	N/A	N/A	
<b>National Synchrotron Light Source-II, BNL</b>	<b>\$56,900</b>	<b>\$56,900</b>	<b>\$90,415</b>	<b>\$110,000</b>	<b>+19,585</b>
Number of Users	0	0	200	700	+500
Achieved operating hours	N/A	N/A	N/A	N/A	
Planned operating hours	0	0	2,100	3,250	+1,150
Optimal hours	0	0	2,300	3,300	+1,000
Percent optimal hours	N/A	N/A	91.3%	98.5%	
Unscheduled downtime hours	N/A	N/A	<10%	N/A	
<b>Stanford Synchrotron Radiation Lightsource</b>	<b>\$38,400</b>	<b>\$38,400</b>	<b>\$39,000</b>	<b>\$40,755</b>	<b>+1,755</b>
Number of Users	1,556	1,556	1,500	1,550	+50
Achieved operating hours	5,176	5,176	N/A	N/A	
Planned operating hours	5,400	5,400	5,200	5,300	+100
Optimal hours	5,400	5,400	5,400	5,400	0
Percent optimal hours	95.9%	95.9%	96.3%	98.1%	
Unscheduled downtime hours	<10%	<10%	<10%	<10%	

	<b>FY 2014 Enacted</b>	<b>FY 2014 Current</b>	<b>FY 2015 Enacted</b>	<b>FY 2016 Request</b>	<b>FY 2016 vs. FY 2015</b>
<b>Linac Coherent Light Source</b>	<b>\$125,050</b>	<b>\$125,050</b>	<b>\$126,956</b>	<b>\$132,669</b>	<b>+5,713</b>
Number of Users	612	612	580	580	0
Achieved operating hours	4,380	4,380	N/A	N/A	
Planned operating hours	4,400	4,400	4,700	4,600	-100
Optimal hours	4,500	4,500	4,700	4,700	0
Percent optimal hours	97.3%	97.3%	100%	97.9%	
Unscheduled downtime hours	<10%	<10%	<10%	<10%	
<b>High Flux Isotope Reactor</b>	<b>\$59,750</b>	<b>\$59,750</b>	<b>\$60,688</b>	<b>\$63,419</b>	<b>+2,731</b>
Number of Users	453	453	450	450	0
Achieved operating hours	3,682	3,682	N/A	N/A	
Planned operating hours	3,400	3,400	3,400	3,450	+50
Optimal hours	3,500	3,500	3,500	3,500	0
Percent optimal hours	105.2%	105.2%	97.1%	98.6%	
Unscheduled downtime hours	<10%	<10%	<10%	<10%	
<b>Lujan Neutron Scattering Center</b>	<b>\$8,900</b>	<b>\$8,900</b>	<b>\$2,000</b>	<b>\$2,000</b>	<b>0</b>
Number of Users	187	187	0	0	0
Achieved operating hours	1,683	1,683	N/A	N/A	
Planned operating hours	1,300	1,300	0	0	0
Optimal hours	2,000	2,000	0	0	0
Percent optimal hours	84.2%	84.2%	N/A	N/A	
Unscheduled downtime hours	<10%	<10%	N/A	N/A	
<b>Spallation Neutron Source</b>	<b>\$178,600</b>	<b>\$178,600</b>	<b>\$181,425</b>	<b>\$189,571</b>	<b>+8,146</b>
Number of Users	866	866	800	850	+50
Achieved operating hours	4,424	4,424	N/A	N/A	
Planned operating hours	4,400	4,400	4,700	4,650	-50
Optimal hours	4,500	4,500	4,700	4,700	0
Percent optimal hours	98.3%	98.3%	100%	98.9%	
Unscheduled downtime hours	<10%	<10%	<10%	<10%	



	FY 2014 Enacted	FY 2014 Current	FY 2015 Enacted	FY 2016 Request	FY 2016 vs. FY 2015
<b>TYPE B FACILITIES<sup>a</sup></b>					
<b>Center for Nanoscale Materials</b>	<b>\$20,100</b>	<b>\$20,100</b>	<b>\$23,427</b>	<b>\$24,481</b>	<b>+1,054</b>
Number of users	451	451	470	500	+30
<b>Center for Functional Nanomaterials</b>	<b>\$19,600</b>	<b>\$19,600</b>	<b>\$19,908</b>	<b>\$20,804</b>	<b>+896</b>
Number of users	473	473	400	420	+20
<b>Molecular Foundry</b>	<b>\$20,150</b>	<b>\$20,150</b>	<b>\$26,403</b>	<b>\$27,591</b>	<b>+1,188</b>
Number of users	433	433	470	500	+30
<b>Center for Nanophase Materials Sciences</b>	<b>\$19,857</b>	<b>\$19,857</b>	<b>\$22,901</b>	<b>\$23,932</b>	<b>+1,031</b>
Number of users	421	421	440	450	+10
<b>Center for Integrated Nanotechnologies</b>	<b>\$20,685</b>	<b>\$20,685</b>	<b>\$21,010</b>	<b>\$21,955</b>	<b>+945</b>
Number of users	465	465	400	420	+20
<b>Total, All Facilities</b>	<b>\$780,692</b>	<b>\$780,692</b>	<b>\$804,948</b>	<b>\$850,832</b>	<b>+45,884</b>
Number of Users	15,749	15,749	13,110	13,970	+860
Achieved operating hours	34,932	34,932	N/A	N/A	
Planned operating hours	33,400	33,400	30,100	31,450	+1,350
Optimal hours	34,700	34,700	30,900	31,900	+1,000
Percent of optimal hours <sup>b</sup>	99.2%	99.2%	97.9%	98.7%	
Unscheduled downtime hours	<10%	<10%	<10%	<10%	

<sup>a</sup> Facility operating hours are not measured at user facilities that do not rely on one central machine

<sup>b</sup> For total facilities only, this is a “funding weighted” calculation FOR ONLY TYPE A facilities:  $\frac{\sum_1^{n1}[(\%OH \text{ for facility } n) \times (\text{funding for facility } n \text{ operations})]}{\text{Total funding for all facility operations}}$

**Scientific Employment**

	<b>FY 2014 Enacted</b>	<b>FY 2014 Current</b>	<b>FY 2015 Enacted</b>	<b>FY 2016 Estimate</b>	<b>FY 2016 vs. FY 2015</b>
Number of permanent Ph.D.'s (FTEs)	4,440	4,440	4,300	4,370	+70
Number of postdoctoral associates (FTEs)	1,160	1,160	1,110	1,130	+20
Number of graduate students (FTEs)	1,730	1,730	1,670	1,690	+20
Other <sup>a</sup>	2,930	2,930	2,840	2,890	+50

<sup>a</sup> Includes technicians, support staff, and similar positions.

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

**1. Significant Changes and Summary**

**Significant Changes**

This Construction Project Data Sheet (CPDS) is an update of the FY 2015 CPDS and does not include a new start for the budget year.

In February 2014, the Office of Science conducted an external Independent Project Review (IPR) as part of the CD-1 development and re-approval process. The IPR committee endorsed the CD-1 cost range of \$750,000,000-\$1,200,000,000, but noted that the project contingency level is lower than that of other comparably scaled projects. Since then, Basic Energy Sciences (BES) has worked with the project to further evaluate the project work scope and cost estimate in response to the IPR. In July 2014, BES revised the preliminary TPC point estimate from \$895,000,000 to \$965,000,000 to include the cost of removing the existing linac in the first kilometer of the tunnel, utility and equipment upgrades needed to support the new superconducting linac and high repetition rate operation, and additional project contingency to reduce risk. Long-lead procurement items will be executed under CD-3B. The milestone dates have been adjusted to reflect this change, which will increase efficiency and further reduce risk.

**Summary**

The most recent DOE 413.3B approved Critical Decision (CD) is a revised CD-1 (Approve Alternative Selection and Cost Range) that was approved on August 22, 2014, with a preliminary TPC range of \$750,000,000-\$1,200,000,000.

A Federal Project Director has been assigned to this project and has approved this CPDS.

The revised LCLS-II project will construct a new high repetition rate electron injector and replace the first kilometer of the existing 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. 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. The revised project will require a cryogenic plant to cool the linac to superconducting temperatures. A 10,000 square foot building will be constructed to house the cryogenic equipment.

An updated Acquisition Strategy was prepared in support of reapproval of CD-1. FY 2014 funding continued design work, R&D, prototyping activities, and fabrication of technical equipment. FY 2015 activities include design, long lead procurements of cryogenic systems, advance procurements of technical materials (primarily niobium), R&D, prototyping, fabrication, and installation activities. FY 2016 funding will continue activities for design, R&D, prototyping, fabrication, and installation, and initiate construction activities.

**2. Critical Milestone History**

(fiscal quarter or date)

	CD-0	Conceptual Design Complete	CD-1	CD-2	Final Design Complete	CD-3	D&D Complete	CD-4
FY 2013	4/22/2010		10/14/2011	1Q FY 2013	4Q FY 2016	3Q FY 2013	N/A	4Q FY 2019
FY 2014	4/22/2010		10/14/2011	4Q FY 2013	4Q FY 2016	4Q FY 2013	N/A	4Q FY 2019
FY 2015 <sup>a</sup>	4/22/2010		10/14/2011	4Q FY 2015	4Q FY 2017	4Q FY 2016	N/A	4Q FY 2021
FY 2016	4/22/2010	1/21/2014	8/22/2014	2Q FY 2016	4Q FY 2017	2Q FY 2016	N/A	4Q FY 2021

<sup>a</sup> This project is pre-CD-2; the estimated cost and schedule are preliminary. Construction will not be executed without appropriate CD approvals.

**CD-0** – Approve Mission Need for a construction project with a conceptual scope and cost range

**Conceptual Design Complete** – Actual date the conceptual design was completed (if applicable)

**CD-1** – Approve Design Scope and Project Costs and Schedule Ranges

**CD-2** – Approve Project Performance Baseline

**Final Design Complete** – Estimated/Actual date the project design will be/was complete (d)

**CD-3** – Approve Start of Construction

**D&D Complete** – Completion of D&D work

**CD-4** – Approve Start of Operations or Project Closeout

	Performance Baseline Validation	CD-3A	CD-3B
FY 2013	1Q FY 2013	3/14/2012	
FY 2014	4Q FY 2013	3/14/2012	
FY 2015	4Q FY 2015	3/14/2012	
FY 2016	2Q FY 2016	3/14/2012 <sup>a</sup>	3Q FY 2015

**CD-3A** – Approve Long-Lead Procurements, Original Scope

**CD-3B** – Approve Long-Lead Procurements, Revised Scope

### 3. Project Cost History

(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	N/A	20,000	405,000
FY 2014	18,000	367,000	385,000	20,000	N/A	20,000	405,000
FY 2015 <sup>b,c</sup>	47,000	799,400	846,400	48,600	N/A	48,600	895,000
FY 2016 <sup>c,d</sup>	47,000	869,400	916,400	48,600	N/A	48,600	965,000

### 4. Project Scope and Justification

#### Scope

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 Linac Coherent Light Source (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, providing up to 10<sup>12</sup> 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 by 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.

<sup>a</sup> CD-3A was approved as part of the original project scope prior to the July 2013 BESAC recommendation. All original project scope long lead procurement work was suspended.

<sup>b</sup> This project is pre-CD-2; the estimated cost and schedule are preliminary. Construction will not be executed without appropriate CD approvals.

<sup>c</sup> Includes MIE funding of \$7,000,000 for the design phase and \$60,000,000 for the construction phase, 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.

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. It 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 revised LCLS-II project based on the July 2013 Basic Energy Sciences Advisory Committee (BESAC) report 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 revised project will require a cryogenic plant to cool the linac to superconducting temperatures. A 10,000 square foot building will be constructed to house the cryogenic equipment.

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 1 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. 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 developed 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.

Prior to implementing the revised LCLS-II project, the original LCLS-II scope included construction of the Sector 10 Annex with a total cost of \$8.2M. The construction costs are included in the preliminary Total Project Cost of \$965M.

### **Justification**

The LCLS-II project’s purpose is to expand the x-ray spectral operating range and the user capacity of the existing 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 here 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.

Based on the factors described above, the most effective and timely approach for DOE to meet the Mission Need and realize the full potential of the LCLS is upgrading the existing x-ray free electron laser at SLAC with a new superconducting accelerator and x-ray sources.

The project has an exemption from the project management requirements in DOE O 413.3B, Program and Project Management for the Acquisition of Capital Assets; however, the project is being conducted in accordance with the project management requirements in DOE O 413.3B, and all appropriate project management requirements have been met.

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)
<b>Superconducting linac-based FEL system</b>		
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 <sup>a</sup> )	$10^9$ (10x spontaneous @ 2.5 keV)	$> 10^{11}$ @ 2.5 keV
<b>Normal conducting linac-based system</b>		
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 <sup>a</sup> )	$10^{10}$ (10x spontaneous @ 13 keV)	$> 10^{12}$ @ 13 keV

<sup>a</sup> 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
<b>Total Estimated Cost (TEC)</b>			
Design phase			
MIE funding			
FY 2012	2,000	2,000	2,000
FY 2013 <sup>a</sup>	5,000	5,000	5,000
<b>Total, MIE funding</b>	<b>7,000</b>	<b>7,000</b>	<b>7,000</b>
Line item construction funding			
FY 2014	4,000	4,000	3,500
FY 2015	21,000	21,000	20,000
FY 2016	15,000	15,000	14,500
FY 2017	0	0	2,000
<b>Total, Line item construction funding</b>	<b>40,000</b>	<b>40,000</b>	<b>40,000</b>
<b>Total, Design phase</b>	<b>47,000</b>	<b>47,000</b>	<b>47,000</b>
Construction phase			
MIE funding			
FY 2012	42,500 <sup>b</sup>	20,000	13,862
FY 2013 <sup>f</sup>	17,500	40,000	27,285
FY 2014	0	0	12,256
FY 2015	0	0	6,597
<b>Total, MIE funding</b>	<b>60,000</b>	<b>60,000</b>	<b>60,000</b>
Line item construction funding			
FY 2014	71,700	71,700	18,713
FY 2015	117,700	117,700	136,387
FY 2016	185,300	185,300	180,300
FY 2017	189,100	189,100	176,000
FY 2018	176,000	176,000	186,000
FY 2019	69,600	69,600	68,700
FY 2020	0	0	43,300
<b>Total, Line item construction funding</b>	<b>809,400</b>	<b>809,400</b>	<b>809,400</b>
<b>Total, Construction phase</b>	<b>869,400</b>	<b>869,400</b>	<b>869,400</b>

<sup>a</sup> FY 2013 funding was requested as a line item, but due to a Continuing Resolution, FY 2013 funds were executed as an MIE.

<sup>b</sup> 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.

(dollars in thousands)

	Appropriations	Obligations	Costs
<b>TEC</b>			
MIE funding			
FY 2012	44,500 <sup>b</sup>	22,000	15,862
FY 2013 <sup>a</sup>	22,500	45,000	32,285
FY 2014	0	0	12,256
FY 2015	0	0	6,597
Total, MIE funding	67,000	67,000	67,000
Line item construction funding			
FY 2014	75,700	75,700	22,213
FY 2015	138,700	138,700	156,387
FY 2016	200,300	200,300	194,800
FY 2017	189,100	189,100	178,000
FY 2018	176,000	176,000	186,000
FY 2019	69,600	69,600	68,700
FY 2020	0	0	43,300
Total, Line item construction funding	849,400	849,400	849,400
Total, TEC <sup>a</sup>	916,400	916,400	916,400

**Other Project Cost (OPC)**

## OPC except D&amp;D

## MIE funding

FY 2010	1,126	1,126	938
FY 2011	9,474	9,474	8,033
FY 2012	8,000	8,000	8,893
FY 2013 <sup>b</sup>	0	0	116
FY 2014	0	0	439
FY 2015	0	0	181

Total, MIE funding	18,600	18,600	18,600
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<sup>a</sup> This project has not yet received CD-2 approval; funding and cost 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.

<sup>b</sup> FY 2013 funding was requested as a line item, but due to a Continuing Resolution, FY 2013 funds were executed as an MIE.



(dollars in thousands)			
	Appropriations	Obligations	Costs
Line item construction funding			
FY 2014	10,000	10,000	8,142
FY 2015	9,300	9,300	2,858
FY 2016	0	0	4,000
FY 2017	0	0	4,300
FY 2018	5,900	5,900	5,700
FY 2019	4,800	4,800	4,300
FY 2020	0	0	700
Total, Line item construction funding	30,000	30,000	30,000
Total, OPC	48,600	48,600	48,600
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	30,000	24,755
FY 2013 <sup>a</sup>	22,500	45,000	32,401
FY 2014	0	0	12,695
FY 2015	0	0	6,778
Total, MIE funding	85,600	85,600	85,600
Line item construction funding			
FY 2014	85,700	85,700	30,355
FY 2015	148,000	148,000	159,245
FY 2016	200,300	200,300	198,800
FY 2017	189,100	189,100	182,300
FY 2018	181,900	181,900	191,700
FY 2019	74,400	74,400	73,000
FY 2020	0	0	44,000
Total, Line item construction funding	879,400	879,400	879,400
Total, TPC <sup>b</sup>	965,000	965,000	965,000

#### 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	37,770	N/A

<sup>a</sup> FY 2013 funding was requested as a line item, but due to a Continuing Resolution, FY 2013 funds were executed as an MIE.

<sup>b</sup> This project has not yet received CD-2 approval; funding and cost 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)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Contingency	9,230	9,230	N/A
Total, Design	47,000	47,000	N/A
Construction			
Site Preparation	24,700	4,700	N/A
Equipment	564,800	564,800	N/A
Other Construction	58,500	38,500	N/A
Contingency	221,400	191,400	N/A
Total, Construction	869,400	799,400	N/A
Total, TEC	916,400	846,400	N/A
Contingency, TEC	230,630	200,630	N/A
Other Project Cost (OPC)			
OPC except D&D			
Conceptual Planning	1,980	1,980	N/A
Conceptual Design	23,658	23,658	N/A
Research and Development	1,972	1,972	N/A
Start-Up	11,550	11,550	N/A
Contingency	9,440	9,440	N/A
Total, OPC	48,600	48,600	N/A
Contingency, OPC	9,440	9,440	N/A
Total, TPC <sup>a</sup>	965,000	895,000	N/A
Total, Contingency	240,070	210,070	N/A

### 7. Schedule of Appropriations Requests

(\$K)

Request		Prior Years	FY 2015	FY 2016	FY 2017	FY 2018	FY 2019	FY 2020	Outyears	Total
FY 2012 (MIE)	TEC	22,000	TBD	TBD	TBD	TBD	TBD	TBD	TBD	TBD
	OPC	18,600	TBD	TBD	TBD	TBD	TBD	TBD	TBD	TBD
	TPC	40,600	TBD	TBD	TBD	TBD	TBD	TBD	TBD	TBD
FY 2013 <sup>b</sup> (MIE)	TEC	165,800	94,000	105,300	19,900	0	0	0	0	385,000
	OPC	19,300	0	700	0	0	0	0	0	20,000
	TPC	185,100	94,000	106,000	19,900	0	0	0	0	405,000
FY 2014	TEC	162,000	122,500	100,500	0	0	0	0	0	385,000
	OPC	19,300	0	700	0	0	0	0	0	20,000
	TPC	181,300	122,500	101,200	0	0	0	0	0	405,000

<sup>a</sup> This project has not yet received CD-2 approval; funding and cost 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.

<sup>b</sup> FY 2013 funding was requested as a line item, but due to a Continuing Resolution, FY 2013 funds were executed as an MIE.

Request	Prior Years	FY 2015	FY 2016	FY 2017	FY 2018	FY 2019	FY 2020	Outyears	Total	
FY 2015 <sup>a</sup>	TEC	142,700	138,700	204,000	185,100	156,000	19,900	0	0	846,400
	OPC	28,600	9,300	0	0	5,900	4,800	0	0	48,600
	TPC	171,300	148,000	204,000	185,100	161,900	24,700	0	0	895,000
FY 2016 <sup>n</sup>	TEC	142,700	138,700	200,300	189,100	176,000	69,600	0	0	916,400
	OPC	28,600	9,300	0	0	5,900	4,800	0	0	48,600
	TPC	171,300	148,000	200,300	189,100	181,900	74,400	0	0	965,000

### 8. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy (fiscal quarter or date)	4QFY2020
Expected Useful Life (number of years)	25
Expected Future Start of D&D of this capital asset (fiscal quarter)	4QFY2045

#### (Related Funding Requirements)

	Annual Costs		Life Cycle Costs	
	Current Total Estimate	Previous Total Estimate	Current Total Estimate	Previous Total Estimate
Operations and Maintenance	\$38.6M	N/A	\$1,317.0M	N/A

The numbers presented are the incremental lifecycle operations and maintenance costs above the existing LCLS. The estimate will be updated and additional details provided after CD-2.

### 9. D&D Information

The new area being constructed in this project is not replacing existing facilities.

	Square Feet
New area being constructed by this project at SLAC .....	10,000
Area of D&D in this project at SLAC .....	0
Area at SLAC to be transferred, sold, and/or D&D outside the project including area previously "banked" .....	10,000
Area of D&D in this project at other sites .....	0
Area at other sites to be transferred, sold, and/or D&D outside the project including area previously "banked" .....	0
Total area eliminated .....	10,000

<sup>a</sup> This project has not yet received CD-2 approval; funding and cost 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.

Prior to implementing the revised LCLS-II project, the original LCLS-II scope included construction of the Sector 10 Annex. This facility is 2,275 ft<sup>2</sup> and was offset by demolition of a 1,630 ft<sup>2</sup> building with the balance offset using banked space. The information above reflects only the new construction associated with the revised project.

### **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.

SLAC is partnering 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 and other similar facilities, 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 from the LCLS Project and other similar facilities will be exploited fully in planning and executing LCLS-II.