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 for achieving 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 2017 Budget Request

The BES FY 2017 Request includes increases for core research and the Energy Frontier Research Centers (EFRCs) in key areas related to Departmental priorities, such as topics in support of the 2015 Quadrennial Energy and Technology Reviews, the Departmental crosscuts, and priorities outlined in the 2015 Basic Energy Sciences Advisory Committee Report, "Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science." A new activity is initiated in Computational Chemical Sciences to leverage U.S. leadership in computational chemistry codes in preparation for exascale computing; this systematic effort to modify or replace existing computational chemistry codes with codes that are well-adapted to anticipated exascale architectures is essential to maintain U.S. leadership in this high impact competitive area. The Request also continues support for the Batteries and Energy Storage Energy Innovation Hub, the Fuels from Sunlight Energy Innovation Hub, and Computational Materials Sciences at the FY 2016 Enacted level.

Toward enabling advancement of clean energy technologies, the BES FY 2017 Request increases support for applicable fundamental research directions. Among these investments, studies of materials and chemistry in extreme environments will analyze key dynamics of phenomena that are central to sustainable clean energy technologies, such as non-equilibrium material response and degradation and the decay and separation of heavy elements and their isotopes in nuclear waste. Research on chemistry and materials for energy efficiency will target a wide range of processes for clean energy utilization and conversion, such as photocatalysis, solar energy conversion, biomimetic catalysis, and thermal conversion materials.

In FY 2017, BES will support optimal operations at all of its scientific user facilities, including support for clean energy research. The Linac Coherent Light Source-II project will continue construction activities, and the Advanced Photon Source-Upgrade Major Item of Equipment (MIE) project is flat funded. FY 2016 is the last year of funding for the NSLS-II Experimental Tools (NEXT) MIE project; no funds are requested in FY 2017. As part of the Presidential BRAIN Initiative and in close coordination with the National Institutes of Health, BES will develop next generation tools and technologies at DOE X-ray Light Sources and Nanoscale Science Research Centers to enable advances in brain imaging and sensing.

In the FY 2017 Request, most funding for the DOE Working Capital Fund (WCF) is transferred to Science Program Direction to establish a consolidated source of funding for goods and services provided by the WCF. The Department's CyberOne project is still funded through program dollars in the Office of Science (SC) Safeguards and Security program. In FY 2016 and prior years, SC WCF costs were shared by SC research programs and Science Program Direction.

The BES FY 2017 Budget Request includes increases for research related to three Department-wide crosscutting activities: Subsurface Science, Technology and Engineering R&D (Subsurface), the Exascale Computing Initiative (ECI), and Advanced Materials for Energy Innovation as described below.

- *Advanced Materials (Adv Mat)* – As part of the Advanced Materials for Energy Innovation crosscut, BES will initiate new research activities to understand materials challenges in the areas of lightweight structural materials, corrosion-resistant materials in extreme environments, and quantum materials. The expanded research will emphasize interfaces in lightweight materials and corrosion, development of new characterization tools and predictive capabilities to design improved chemistries and structures, and discovery of new quantum materials with unprecedented properties. These priorities were identified in the 2015 Quadrennial Technology Review, with research directions supported by BES basic research needs reports and the 2015 BES Advisory Committee report "Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science."

- *Exascale Computing Initiative (ECI)* – As part of the ECI, BES will be responsible for the Computational Materials Sciences activity and will initiate a new Computational Chemical Sciences activity in FY 2017. Collectively, Computational Materials and Chemical Sciences will support basic research resulting in codes to predictively design functional materials and chemical processes, 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 (2010), and the follow-on community-based workshops that occurred in 2011–2015 identified a number of applications that would take full advantage of future exascale computing resources, including: 1) new catalysts to improve the efficiency of industrial processes, make effective use of bioenergy, drive energy conversion processes, and mitigate environmental impact; 2) better models of photovoltaic processes and improved efficiency of photovoltaic devices; 3) natural and artificial photosynthesis to unlock the potential of solar driven energy conversion and storage; 4) next generation electronic and magnetic materials whose properties are governed by the strong interactions of electrons and have totally new functionalities; 5) membranes and molecular complexes composed of solid-gas/liquid interfaces, which are critical for separation technologies for energy and water applications.

- *Subsurface Science, Technology and Engineering R&D (Subsurface)* – In FY 2015, BES organized and participated in two strategic planning activities that identified a grand challenge for subsurface science: "Advanced imaging of geophysical and geochemical signals in the subsurface." BES will initiate new Energy Frontier Research Centers in FY 2017 to support multidisciplinary teams to address this grand challenge. The scientific focus will be on fracture networks, associated fluid flow and reaction, and the gaps in fidelity, resolution, and conceptual understanding of subsurface imaging in hard-to-access environments. In addition, BES will support single investigator research on fundamental geochemistry and geophysics with an emphasis on subsurface fluid flow and complex chemistry on widely varying timescales from microseconds to millennia. This research is anticipated to have high relevance for oil and gas production, geothermal energy applications, carbon capture and storage, and nuclear waste disposal.

FY 2017 Crosscuts ($K)

	Subsurface	ECI	Adv Mat	Total
Basic Energy Sciences	41,300	26,000	17,600[a]	84,900

[a] This $17,600K supports the Department's Advanced Materials Crosscut. An additional $11,500K in BES for Quantum Materials is also included in SC's total investment, as described in the advanced materials crosscut narrative.

Basic Energy Sciences
Funding ($K)

	FY 2015 Enacted	FY 2015 Current[a]	FY 2016 Enacted	FY 2017 Request[b]	FY 2017 vs FY 2016
Materials Sciences and Engineering					
Scattering and Instrumentation Sciences Research	64,407	67,788	62,260	70,318	+8,058
Condensed Matter and Materials Physics Research	122,120	120,539	118,049	133,800	+15,751
Materials Discovery, Design, and Synthesis Research	72,424	70,882	70,010	76,871	+6,861
Experimental Program to Stimulate Competitive Research (EPSCoR)	9,951	9,951	14,776	8,520	-6,256
Energy Frontier Research Centers (EFRCs)	50,800	50,800	55,800	55,800	0
Energy Innovation Hubs—Batteries and Energy Storage	24,175	24,175	24,137	24,088	-49
Computational Materials Sciences	8,000	8,000	12,000	12,000	0
SBIR/STTR	12,008	0	12,758	14,448	+1,690
Total, Materials Sciences and Engineering	**363,885**	**352,135**	**369,790**	**395,845**	**+26,055**
Chemical Sciences, Geosciences, and Biosciences					
Fundamental Interactions Research	76,796	73,429	74,599	79,233	+4,634
Chemical Transformations Research	93,493	91,000	92,341	106,423	+14,082
Photochemistry and Biochemistry Research	68,797	73,735	64,189	71,197	+7,008
Energy Frontier Research Centers (EFRCs)	49,200	49,200	54,200	86,766	+32,566
Energy Innovation Hubs—Fuels from Sunlight	15,000	15,000	15,000	15,000	0
Computational Chemical Sciences	0	0	0	13,635	+13,635
General Plant Projects (GPP)	600	1,000	1,000	1,000	0
SBIR/STTR	10,350	0	10,732	14,102	+3,370
Total, Chemical Sciences, Geosciences, and Biosciences	**314,236**	**303,364**	**312,061**	**387,356**	**+75,295**
Scientific User Facilities					
Synchrotron Radiation Light Sources	447,186	450,103	481,906	489,059	+7,153
High-Flux Neutron Sources	244,113	245,050	264,645	261,177	-3,468
Nanoscale Science Research Centers (NSRCs)	113,649	114,925	118,763	122,272	+3,509
Other Project Costs	9,300	9,300	0	0	0
Major Items of Equipment	42,500	42,500	35,500	20,000	-15,500
Research	31,713	26,847	34,853	37,537	+2,684
SBIR/STTR	27,918	0	31,182	33,484	+2,302
Total, Scientific User Facilities	**916,379**	**888,725**	**966,849**	**963,529**	**-3,320**
Subtotal, Basic Energy Sciences	**1,594,500**	**1,544,224**	**1,648,700**	**1,746,730**	**+98,030**

[a] Reflects the transfer of Small Business Innovation/Technology Transfer Research (SBIR/STTR) funds within the Office of Science.
[b] A transfer of $3,867,000 to Science Program Direction is to consolidate all Working Capital Funds in one program.

	FY 2015 Enacted	FY 2015 Current[a]	FY 2016 Enacted	FY 2017 Request[b]	FY 2017 vs FY 2016
Construction					
Linac Coherent Light Source-II (LCLS-II), SLAC	138,700	138,700	200,300	190,000	-10,300
Total, Construction	**138,700**	**138,700**	**200,300**	**190,000**	**-10,300**
Total, Basic Energy Sciences	**1,733,200**	**1,682,924**	**1,849,000**	**1,936,730**	**+87,730**

SBIR/STTR Funding:

- FY 2015 Transferred: SBIR $44,182,000 and STTR $6,094,000
- FY 2016 Projected: SBIR $47,540,000 and STTR $7,132,000
- FY 2017 Request: SBIR $54,385,000 and STTR $7,649,000

Basic Energy Sciences
Explanation of Major Changes ($K)

	FY 2017 vs FY 2016 Enacted
Materials Sciences and Engineering: Additional funds are requested to support research in areas identified as high priorities in the Quadrennial Technology Review, the Departmental crosscuts, and the 2015 BES Advisory Committee report "Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science." A major emphasis is an increase in materials research under extremes of temperature, pressure, stress, photon and radiation flux, electromagnetic fields, and electrochemical environments often encountered in clean energy technologies. Additional research will support novel materials for enhanced efficiency in energy conversion and utilization. Topical areas cover light-weight composites, thermoelectric and thermocaloric materials for efficient heat conversion, and quantum materials for next generation electronics. There will be an increase in synthesis science underpinning these enhanced activities. Specifically, the research will target the development of the understanding required for predictive design of interfaces in lightweight polymer composite materials that are relevant to efficient energy systems and transportation; to determine the mechanisms of corrosion in radiative and other extreme chemical/temperature environments relevant to improved energy generation systems; to investigate quantum materials as a foundation for next generation electronics and computing; to study thermal transport in materials to make efficient use of heat; to advance new characterization tools to understand how materials respond and evolve during actual use; and to develop models of materials synthesis that enable understanding of how to control and configure atoms to achieve a desired structure and function.	**+26,055**
Chemical Sciences, Geosciences, and Biosciences: A new initiative in Computational Chemical Sciences will leverage U.S. leadership in computational chemistry codes in preparation for the path to exascale computing. A systematic effort to modify or replace existing computational chemistry codes with codes that are well-adapted to anticipated exascale architectures is critically needed to enable high-fidelity simulations to inform models that improve and accelerate the research, design, demonstration, and deployment phases of the energy innovation cycle. Additional funds are requested to support single investigator and team research related to the Subsurface crosscut. Through the Energy Frontier Research Center (EFRC) program, BES will support multidisciplinary teams to address the grand challenge of "advanced imaging of geophysical and geochemical signals in the subsurface," with a focus on fracture networks, associated fluid flow and reaction, and the gaps in fidelity, resolution, and conceptual understanding of subsurface imaging in hard-to-access environments. In addition, BES will support single investigator research on fundamental geochemistry and geophysics with an emphasis on subsurface fluid flow and complex chemistry on widely varying timescales from microseconds to millennia. Among efforts to enable advances in clean energy technologies, chemistry research will target the areas of energy efficiency and chemistry in extreme environments. Investments in energy efficiency will target the discovery of catalysts with higher activity and selectivity, leading to lower energy consumption for chemical conversions and less demand for the purification of products. BES will support small groups of multidisciplinary investigators to draw on biomimetic and computational expertise, including synergistic approaches such as electro- and photo (electro) catalysis. Chemistry under extreme conditions will focus on the radiative environments generated by energetic photons, electrons and intense x-rays, for example, to understand nuclear waste mixtures. Targeted research will elucidate the nature, dynamics, and kinetics of complex chemical processes ranging from fundamental research on elements with f-electrons to highly selective removal of specific radioactive species.	**+75,295**

	FY 2017 vs FY 2016 Enacted
Scientific User Facilities: BES will support optimal operations at all of the scientific user facilities—five light sources, five Nanoscale Science Research Centers, and two neutron sources—to enable research including clean energy research. FY 2016 is the last year of funding for the NEXT MIE project. In FY 2017, no funds are requested for NEXT or for Other Project Costs for the Linac Coherent Light Source-II (LCLS-II) construction project per the project plan. The Advanced Photon Source-Upgrade MIE project is flat funded. As part of the Presidential BRAIN Initiative and in close coordination with the National Institutes of Health, BES will develop next generation tools and technologies at DOE X-ray Light Sources and Nanoscale Science Research Centers to enable advances in brain imaging and sensing.	**-3,320**
Construction: Funding for the LCLS-II construction project will decrease slightly in FY 2017 per the project plan.	**-10,300**
Total, Basic Energy Sciences	**+87,730**

Basic and Applied R&D Coordination

As a program that supports fundamental scientific research relevant to many Department of Energy mission areas, 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 Energy Innovation Hubs Working Group meets regularly to coordinate programmatic oversight and promote commonality across the Hubs. BES also coordinates with DOE technology offices on the Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) program, including 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 the Advanced Research Projects Agency-Energy (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 crucial role in achieving integration of basic and applied research.

Program Accomplishments

National Synchrotron Light Source-II. The NSLS-II construction project has been completed on time and within budget.

- Construction of the most advanced storage-ring-based light source facility in the world, the National Synchrotron Light Source-II (NSLS-II) at Brookhaven National Laboratory, was completed in March 2015, about 3 months ahead of schedule. The planning, design, and construction of this 627,000-square-foot facility spanned 10 years at a total project cost of $912 million. The project benefited from $150 million of American Recovery and Reinvestment Act funding, which allowed the project to accelerate civil construction and to reduce overall project risks. This premier BES scientific user facility produces extremely bright beams of x-rays, providing unprecedented capabilities to accelerate advances in chemistry, biology, energy, geology, physics, and materials science. NSLS-II has been officially designated as a user facility and started serving general users in July 2015.

Chemistry by Design. Coupling predictive theory and computation with advanced synthesis has led to the discovery of molecular assemblies with novel functions.

- Complementary computational and experimental analyses revealed the interplay of electronic and geometric effects that are responsible for the formation of a new class of nanoscale cage clusters of uranium peroxide. These clusters could be produced under chemically simple conditions and be tailored to selectively bind to toxic or undesirable chemical species, enabling their use in chemical purification and separation for nuclear fuel reprocessing or environmental decontamination.
- In a feat of computational chemistry, researchers bypassed potentially decades of experiments with the results from one day's worth of computing time on the Argonne Leadership Computing Facility supercomputer, Mira. Rather than synthesize hundreds of thousands of catalytic porous zeolites and test each one for their ability to purify ethanol and enhance fuel production, the researchers utilized a hierarchical predictive chemical simulation to predict the most effective zeolitic structure. Synthesis and experimental testing of the predicted zeolitic

framework proved that the simulation produced the "right answer": a new catalyst that is highly effective, with potential to streamline industrial-scale ethanol purification from a multi-step to single-step process.

- Experiments and computation were used to demonstrate that a new compound based on a metal-organic framework (MOF) was effective in degrading soman—one of the most toxic chemical agents—in minutes. The new MOF structure contains nodes of zirconium atoms that selectively break the bond in the nerve agent, rendering it innocuous. While the structural design was inspired by a natural enzyme in bacteria, the new MOF compound is thermally and chemically robust and functions in wide temperature ranges and humid environments.

Cooperative interactions drive new molecular behavior. Complex interactions and correlations of the atomic and molecular constituents in matter have resulted in new chemical properties, expanding the frontiers of energy applications.

- Conversion of nitrogen to ammonia, as in the synthetic Haber-Bosch process, also occurs in natural systems, following a far less energy-intensive pathway. Computational analysis of this pathway in the nitrogenase enzyme of algae and plants revealed that a small iron-based protein "rocks" across the surface of the larger nitrogenase unit during the conversion. The rocking motion pushes the two molecular units into close contact, facilitating the key transfer of electrons. This insight may lead to innovative design principles for a more energy-efficient synthetic process.
- X-ray crystallography showed how the orange carotenoid protein in cyanobacteria may protect plants from photodamage when exposed to sunlight. Researchers observed that under illumination, a carotenoid pigment molecule within the protein moved 12 Ångstroms (approximately 4 atom widths)—an extremely large movement whose scale is unprecedented in observations of this kind. Researchers hypothesized that the movement couples the pigment to the light absorbers in plants, allowing excess light energy to be converted to heat and preventing photodamage. Understanding such interactions that are central to light harvesting and photoprotection can help guide design of stable and efficient artificial photosynthetic systems.
- Experiments and computation have uncovered a novel cooperative mechanism for CO_2 adsorption in porous MOF materials. Insertion of one CO_2 molecule into the MOF facilitates the insertion of another CO_2 at a neighboring site, resulting in a "domino effect" of carbon adsorption along the cylindrical pores of the MOF. This efficient and tunable class of adsorbents may allow for drastic reductions in the capital cost of carbon capture from power plant flue gas or from the atmosphere.

Predictive Materials Science. The Materials Genome Initiative supports the integration of theory and experimental research to accelerate materials discovery. New computer codes and extensive databases for predictive materials science research are now available to the public.

- By harnessing high performance computing and state-of-the-art theoretical tools, computed properties of new and predicted materials have been gathered into a publicly available database for over 60,000 compounds, 70,000 electrochemical phase diagrams, 28,000 electronic band structures, and 1,300 full elastic tensors (for mechanical behavior). These data are being used by over 16,000 scientists and engineers, including over 2,000 from industry, to identify new electrolytes and electrode materials for batteries, thermoelectric materials, and photocatalysts for chemical conversions.
- Through a combination of theory and advanced characterization techniques, the roles of specific element additions to magnesium alloys have been predicted, and then demonstrated via experiments, to promote development of precipitates that optimally control the mechanical properties of the lightweight materials. The results led to new mechanistic understanding on how to make lightweight materials stronger.
- Improved algorithms have been developed for the quantum Monte Carlo method, a computational technique that can predict the quantum state and geometric structure of complex materials for which standard methods fail. The new codes are publicly available and have predicted experimentally-validated binding energies and diffusivities for lithium ion batteries, surface energies for catalysts, volumes and bulk moduli for metals and ionic materials, and melting temperatures of hydrogen under pressure.

Going beyond post-mortem analysis – materials characterization in real time and under real operating conditions. "In situ" or "in operando" characterization investigates materials evolution, leading to more efficient synthesis and discovery of new and improved materials.

- During charging and discharging of a commercial lithium ion battery, a novel, lensless x-ray diffraction technique imaged the structure of a nanoparticle in an electrode and the migration of defects. During extreme charging, phase changes were localized to the material near the defects, providing new understanding that could lead to defect engineering for optimized battery performance.
- Catalysts drive efficient industrial processes for energy production and pollution control. During high-energy x-ray experiments, specific surface characteristics of palladium and nickel nanoparticles were observed to accelerate the conversion of carbon monoxide to CO_2. Analysis of the experiments, combined with theoretical calculations, showed that the number of atomic neighbors at surface sites and the distances between atoms can tune catalytic activity.
- For the first time, nanoparticles rotating freely in a liquid solution have been “seen” in three dimensions (3D) with near-atomic resolution. Images from world-leading electron microscopes, equipped with a graphene-based liquid cell and direct electron detectors, were reconstructed into high-resolution 3D movies of the interactions and growth of platinum nanoparticles. Results confirmed that individual, and surprisingly asymmetric, particles from the same synthesis solution followed different growth pathways, providing a new approach to understand and control growth of nanoparticle structures.

BES user facilities enable U.S. industries to advance frontiers in information and semiconductor technologies.

- An original laser zone annealing apparatus has been constructed at the Center for Functional Nanomaterials that can quickly form self-assembled polymer nanostructures over an 8-inch-diameter semiconductor wafer. The new process reduces the ordering time of the block-copolymer self-assembly by more than 1,000-fold, from hours to less than a second, making this tool extremely attractive for industrial-scale, rapid manufacture of ordered nanoscale arrays for terabyte magnetic memories, nanoelectronics, and nanophotonics.
- The IBM Research Alliance worked with researchers at Argonne National Laboratory to develop a new method for quantitatively mapping the detailed structures of microprocessors at nanoscale spatial resolution. The ability to noninvasively detect and control subtle perturbations of the atomic crystal lattice planes in operating devices is critical to improving the performance and reliability of computer processors. This technique can also be applied to other nanoscale systems such as photovoltaics, power electronics, and batteries.
- Researchers at the Center for Nanoscale Materials transferred their innovative low-temperature diamond deposition technology to the U.S. semiconductor industry. The method deposits nanocrystalline diamond on a variety of wafer substrate materials at temperatures as low as 400°C, enabling for the first time the integration of high-power diamond electronics with conventional silicon integrated circuits.

Neutron scattering enables basic discoveries in magnetism, solving a decades-old conundrum, and facilitates advances critical to performance of fuel injectors and catalytic converters.

- Researchers have discovered time-fluctuating magnetism in the radioactive element plutonium (Pu) using inelastic neutron scattering techniques at the Spallation Neutron Source. The surprising result that the magnetism is not of a conventional static character, but instead rapidly fluctuates in time, resolves a 50-year-old controversy between theory and experiment over the existence of magnetism in Pu.
- Using time-resolved neutron imaging, scientists have observed local fuel flow dynamics of a gasoline injector nozzle. Measurements reveal cavitation and local pressure-drop effects during one-millisecond-long injection events. These first direct observations are critical in developing advanced computational models and in understanding fluid flow processes to improve vehicle fuel efficiency and lower emissions.
- Neutron imaging has been used to measure the distribution of water inside an entire catalytic converter for vehicles. The presence of water can seriously degrade the performance of these converters, and neutron imaging provides a unique insight into how such engineered water-management systems perform in practical operations.

Basic Energy Sciences
Materials Sciences and Engineering

Description

The 2015 Quadrennial Energy and Technology Reviews confirm the continued critical role of materials to nearly every aspect of energy generation and end-use, especially as these challenges relate to clean energy and energy efficiency. Materials limitations are often the barrier to improved energy efficiencies, longer lifetimes of infrastructure and devices, or the introduction of new or cleaner energy technologies. The latest BES Advisory Committee report, "Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science," provided further documentation of the importance of materials sciences in forefront research for next generation scientific and technology advances. The *Materials Sciences and Engineering* subprogram supports research to provide the fundamental understanding of materials synthesis, behavior, and performance that will enable solutions to wide-ranging energy generation and end-use 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, theory/computational, and instrumentation 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, multi-functional nanoporous and mesoporous structures for optimum ionic and electronic transport in batteries and fuel cells, materials with longer lifetimes in extreme environments through better materials design and self-healing processes, and new materials with novel, emergent properties that will open new avenues for technological innovation.

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 and dynamics across multiple length and 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 including electronic, thermal, optical, and mechanical properties.

- **Materials Discovery, Design, and Synthesis**—Developing the knowledge base and synthesis strategies to design and precisely assemble structures to control properties and enable 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, from the nanoscale to mesoscale, and translation of this understanding to prediction of material behavior, transformations, and processes in challenging real-world systems. An example of this research is examination of the transformations that take place in materials with many atomic constituents, complex structures, and a broad range of defects when these materials are exposed to extreme environments – such as those found in fossil energy, nuclear energy, and most industrial settings. To maintain leadership in materials discovery, the research explores new frontiers of unpredicted, emergent materials behavior; utilization of nanoscale control; and materials systems that are metastable or far from equilibrium. Finally, the research includes investigation of the interfaces between physical and biological sciences to explore 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.

Among its efforts toward enabling advancement of clean energy technologies, the subprogram stresses fundamental research related to materials behavior under extreme environments and on materials phenomena that will promote more efficient use and conversion of energy. New materials and their responses under extremes in temperature, pressure, stress, photon and radiation flux, electromagnetic fields, and electrochemical environments are important to future improvements in energy efficiency and for clean generation and use. Advanced characterization tools and instruments across a wide range of space and time scales, especially in combination and under dynamic "in operando" conditions that can analyze non-equilibrium materials and excited-state phenomena, are essential to this work. For thermal energy efficiency, new thermocaloric materials can improve efficiency in cooling and in microelectronic devices, and new thermoelectric materials can convert wasted heat into electricity. New fundamental understanding of heat transport and energy conversion in materials and of the behavior of thermoelectric properties is necessary for these advances. Additional research will target lightweight materials such as polymers and polymer composites, and new families of porous materials of importance for carbon capture technologies.

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 and the associated databases for predictive design of materials.

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. The use of DOE's world-leading electron, neutron, and synchrotron x-ray scattering facilities in major advances in materials science, and by large materials science user communities, is continuing evidence of the importance of this research field. The BES Advisory Committee report, "Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science," identified imaging as one of the pillars for transformational advances for the future.

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 of multiscale phenomena to extract heretofore unattainable information on multiple length and time scales is a growing aspect of this research, as is the use of combined scattering techniques.

Understanding how extreme environments (temperature, pressure, stress, photon and radiation flux, electromagnetic fields, and electrochemicals) impact materials at the atomic and molecular level and cause changes that eventually result in materials failure is required to design transformational new materials for energy-related applications. Advances in characterization tools, including ultrafast techniques, are needed to measure non-equilibrium and excited-state phenomena at the core of the complex, interrelated physical and chemical processes that underlie materials performance in these conditions. Information from these characterization tools is the foundation for the creation of new materials that have extraordinary tolerance and can function within an extreme environment without property degradation.

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 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 of this research program is to characterize and understand materials whose properties are derived from the strong interactions of electrons in their structure, such as unconventional superconductors and magnetic materials. An emerging topic is "quantum materials"—materials whose properties result from strong and coherent interactions of the constituent electrons with each other, the atomic lattice, or light. Emphasis is placed on investigating low-dimensional systems, including nanostructures and two-dimensional layered structures such as graphene, multilayered structures of two-dimensional materials, and studies of the electronic properties of materials at ultra-low temperatures and in 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 the electron spin-phenomena and basic semiconductor physics relevant to next generation electronics and information technologies. 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 advance the theories that are being used to describe material properties across a broad range of length and time scales, from 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.

This activity also emphasizes research to understand how materials respond to their environments, including the influence of temperature, electromagnetic fields, radiation, and corrosive chemicals. This research 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.

The Quadrennial Technology Review identified materials research in this area as critical for additional investments and coordination with the DOE technology programs, especially related to more efficient and cleaner energy generation and use. Three key areas with high potential for accelerated development were identified and are proposed for additional research support: lightweight structural materials, corrosion-resistance for materials use in extreme environments, and quantum materials. A basic research challenge for lightweight materials such as polymer composites is improved understanding of how to design the interfaces between the matrix and the reinforcements, including new tools to characterize these interfaces and predictive capabilities to design improved chemistries and structures. The need for corrosion resistant materials is clear—energy technologies continue to place increasing demands on materials performance with respect to extremes in stress, strain, temperature, chemical reactivity and radiation flux as lifetimes are extended and operating conditions are optimized for maximal efficiency and minimal environmental impact. These operating conditions demand materials that can be used reliably in these extreme environments, requiring a comprehensive understanding of the impact of the degradation that results from exposures to these conditions. Additional research is proposed to assess the evolution of material structure and properties in multiple extreme environments, including multiscale modeling (nano to meso to macro) with emphasis on the interfaces in the materials, often a region with enhanced susceptibility to corrosion and degradation. Many energy-relevant technological advances, ranging from magnetism to superconductivity, are enabled by quantum materials. Due to recent advances in the ability to manipulate and exploit coherence in light and matter, additional research is proposed to take advantage of these phenomena to discover new materials with unprecedented properties. Research would include predictive modeling, evaluation of phenomena that occur at ultrafast timescales (beyond-equilibrium phenomena), and controlled synthesis and design of materials to enable high quality, tailored interfaces, controlled heterogeneity, and coherent manipulation of charge, spin and lattice dynamics that result in entirely new material properties.

In addition, new research will focus on developing a fundamental understanding of materials phenomena related to heat management and use of excess heat for improved thermal efficiency. Important to this research area is improved theoretical understanding of heat transport and energy conversion in materials. Fundamental theory to advance novel materials for high temperature environments, such as high-entropy alloys, will also be emphasized.

<u>Materials Discovery, Design, and Synthesis Research</u>

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 continues to be 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.

The BES Advisory Committee report on transformative opportunities for discovery science reinforced the importance of the continued growth of synthesis science, recognizing the transformational opportunity to realize targeted functionality in materials by controlling the synthesis and assembly of hierarchical architectures and beyond equilibrium matter. Research supported in this portfolio underpins many energy-related technologies such as batteries and fuel cells, catalysis and electrocatalysis, solar energy conversion and storage, friction and lubrication, and filtration membranes and porous architectures for advanced separations, efficient ion transport, and highly selective gas separation and storage. For example, for lighter weight materials, research on polymers and polymer composites generates new insights into the design of idealized matrix-additive interfaces, new chemistries, and exploiting the structural hierarchies to engineer a material's strength and other mechanical properties.

In addition to research on chemical and physical synthesis processes, an important element of this portfolio is research to understand how to use bio-mimetic and bio-inspired approaches to design and synthesize novel materials with some of the unique properties found in nature, e.g., self-repair and adaptability to the changing environment. Major research directions include the controlled synthesis and assembly of nanoscale materials into functional materials with desired properties; porous materials with customized porosities and reactivities; mimicking the energy-efficient, low temperature synthesis approaches of biology to produce materials under mild conditions; bio-inspired materials that assemble autonomously and, in response to external stimuli, dynamically assemble and disassemble to form non-equilibrium structures; and adaptive and resilient materials that also possess self-repairing capabilities. The portfolio also 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, in situ 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.

Related to improved energy efficiency and expansion of the knowledge base for cleaner energy generation and use, thermocaloric and thermoelectric materials is a prominent area that will see significant growth. Another topic of increasing importance is carbon capture technologies, especially the development of new families of porous materials. This research will require a concerted effort in manipulating the pore sizes, gas-solid binding interactions and properties ranging from the mechanical stability to kinetic selectivity.

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 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. The current 32 centers (22 of which were renewed from the initial group, and 10 of which are new centers initiated in FY 2014) continue to expand upon these accomplishments. These EFRCs are 4-year awards with funding for the final two years contingent upon successful outcome of a mid-term review.

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.

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 continues to evolve their 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 science-focused reviews in July 2014 and in July 2015. The review panels provided positive input and recommendations for furthering the JCESR research goals. The July 2015 review reported significant progress towards the project goals. BES continues to monitor progress closely. FY 2017 is the last year of the first award period for JCESR. The fifth year of research ends in December 2017. Evaluations of research progress in FY 2016 and FY 2017 will be used to determine if renewal of JCESR will be considered, including assessment of the funding level and technical focus for a renewal award.

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.

This paradigm shift will 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.[a] Examples include dynamics and strongly correlated matter, conversion of solar energy to electricity, design of new catalysts for a wide range of industrial uses, and transport in materials for improved electronics. Success will require extensive research and development with the goal of creating experimentally validated, robust community codes that will enable functional materials innovation.

Research awards to perform computational materials research were launched in FY 2015 (3 teams) and additional awards (up to 2 additional teams) will be supported in FY 2016. The 4-year awards focus on creation of computational codes and associated experimental/computational databases for the design of functional materials. This research is performed by fully integrated teams, combining the skills of experts in materials theory, modeling, computation, synthesis, characterization, and processing/fabrication. 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 to validate computational models, and well-controlled synthesis to confirm the predictions of the codes. Research uses the unique world leading tools and instruments at DOE's user facilities, from ultrafast free electron lasers to aberration-corrected electron microscopes and instrumentation for atomically controlled synthesis. The computational codes will advance the predictive capability for functional materials, use DOE's leadership class computational capabilities, and be positioned to take advantage of future exascale leadership class computers. The ideal end products for this research are publicly accessible databases of experimental/computational data and open source, robust, validated, user friendly software that captures the essential physics and chemistry of relevant materials systems. The ultimate goal is use of these codes/data by the broader research community and by industry to dramatically accelerate the design of new functional materials.

FY 2017 funding will continue support of the teams that received multi-year awards in FY 2015 and those awarded in FY 2016 to perform the basic research and develop/deliver codes and associated experimental/computational data for the design of functional materials. Computational materials science research activities are managed using the approaches developed by BES for similar large team funded modalities. Management reviews by a peer review panel are held in the first year of the award, followed by a mid-term peer review to assess scientific progress, with monthly teleconferences, quarterly and annual progress reports, and active management by BES throughout the performance period.

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

Activities and Explanation of Changes

FY 2016 Enacted	FY 2017 Request	Explanation of Changes FY 2017 vs FY 2016
Materials Sciences and Engineering $369,790,000	**$395,845,000**	**+$26,055,000**
Scattering and Instrumentation Sciences Research $62,260,000	**$70,318,000**	**+$8,058,000**
Research continues to emphasize use of advanced characterization techniques to tackle forefront science on energy-relevant materials science phenomena. Ultrafast science continues to be a priority research area. Investments will emphasize hypothesis-driven research with existing ultrafast science capabilities, including lab-based and x-ray free electron laser sources, to establish a more complete understanding of materials properties and behaviors. Neutron scattering sciences 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 *in situ* analysis capabilities under perturbing parameters such as temperature, stress, chemical environment, and magnetic and electric fields are pursued. Research that uses traditional diffraction, imaging, and spectroscopy techniques continues at a reduced level.	Research into ultrafast science, including development of electron optics and sources, sample environments, and enhanced detectors will continue to better understand critical dynamic processes at sub-angstrom spatial resolution and nanosecond temporal resolution. The program will stress hypothesis -driven research with existing ultrafast science capabilities. Based on the important role that in operando characterization can play in improving materials for energy-related environments and the BES advisory committee report on transformative challenges for materials discovery, the program will emphasize research that advances imaging with x-rays, neutrons, and electrons to form spatially and temporally resolved maps of dynamics that allow quantitative predictions of time-dependent material properties and chemical processes. New advances in spectroscopy, high-resolution analyses of energy-relevant soft matter, and quantitative *in situ* analysis capabilities under perturbing parameters such as temperature, stress, chemical environment, and magnetic and electric fields will be pursued.	The FY 2017 program will enhance research understanding of imaging with x-rays, neutrons, and electrons to form spatially and temporally resolved maps of dynamics regarding evolution of chemical composition, crystal orientation, structural phases, magnetic and electric domains, cracks, and defects in materials, including evolution in the atomic structure caused by exposure to heat, stress, chemicals, current flow, and other environmental factors associated with materials use, especially as these relate to improving efficient use of energy. Support for materials characterization research that does not elucidate functionality or interrogate phenomena spanning multiple length and time scales will be reduced. Topical areas specifically targeted for reduction include conventional superconductivity, organic photovoltaics, confined nanofluids, and mature use of high pressure scattering, spectroscopy, and imaging. Research involving well-established neutron and x-ray scattering and imaging techniques, and conventional microscopy and scanning probe imaging for studies of materials behavior will be deemphasized.
Condensed Matter and Materials Physics Research $118,049,000	**$133,800,000**	**+$15,751,000**
The program continues to support fundamental experimental and theoretical research on the properties of materials. It focuses on structural, optical, and electrical properties and control of material functionality in response to external stimuli	The program will continue to support experimental and theoretical research that advances our fundamental understanding of known materials and will lead to the discovery of new materials and new phenomena. The program will initiate research	For structural materials, additional research will focus on lightweight polymer composites, emphasizing design of the matrix-reinforcement interfaces, including new characterization tools and predictive capabilities to design improved chemistries and

FY 2016 Enacted	FY 2017 Request	Explanation of Changes FY 2017 vs FY 2016
including temperature, pressure, magnetic and electric fields, and radiation. Phenomena in materials are investigated from atomistic through nanoscale to mesoscale length scales. The research supported continues 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, are continued. Research involving theory and computational data coupled to experimental characterization of material properties continues to grow. Research on superconducting vortex matter, isolated nanoparticles, quantum Hall behavior, and low dimensional phenomena in carbon nanotubes and graphene continues at a reduced level.	activities related to more efficient and cleaner energy as identified in the Quadrennial Energy and Technology Reviews. Also, it will initiate research with a focus on lightweight structural materials, corrosion, and quantum materials—materials whose properties result from strong and coherent interactions of the constituent electrons with each other, the atomic lattice, or light. Research on lightweight structural materials and corrosion resistant materials, especially those exposed to extreme stress, strain, temperature, reactive chemicals and radiation flux, will focus on development of understanding of interfacial phenomena and on predictive design capabilities. Research will expand on thermal transport in materials, including caloric, high entropy, and high temperature materials and non-dissipative transport in novel topological materials.	structures. For materials in extreme environments, additional research will emphasize the development of a fundamental understanding of corrosion and degradation processes including the role of interfaces, linking nano/microscale and mesoscale phenomena, and development of quantitative prediction capabilities for materials performance in multiple extreme conditions. In the area of quantum materials, research will focus on predictive modeling, evaluation of ultrafast regimes (non-equilibrium phenomena), and controlled synthesis and design of materials to enable high quality, tailored interfaces, controlled heterogeneity, and coherent manipulation of charge, spin and lattice dynamics. The program will continue to deemphasize research on granular materials, conventional superconductivity, high strain rate, high dose radiation effects, and cold atom physics. It will continue to reduce research on superconducting vortex matter and heavy fermion phenomena; isolated nanoparticles and quantum dots; quantum wells; and quantum Hall behavior. Studies on low dimensional phenomena in carbon nanotubes and single-layer graphene will continue to be reduced in favor of research that involves interactions of nano and low dimensional systems that can potentially produce new phenomena with properties related to advanced energy technologies.
Materials Discovery, Design, and Synthesis Research **$70,010,000**	**$76,871,000**	**+$6,861,000**
Research continues to focus on the predictive design and synthesis of materials across multiple length scales 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, are developed. Additionally,	Research on “Synthesis Science”, i.e., predictive materials design and synthesis, will expand to accelerate the pace of discovery of new materials as well as to provide a foundation for next generation energy technologies. In addition, the program will increase focus on fundamental materials synthesis and materials chemistry related to improved energy	The increase will support research related to energy-efficient use of heat, such as thermocaloric and thermoelectric materials, improved polymer chemistries to control interfaces related to light weight polymer composites, and discovery of new classes of porous materials and improved catalysts. Additional research will exploit advances in characterization of

FY 2016 Enacted	FY 2017 Request	Explanation of Changes FY 2017 vs FY 2016
synthesis pathways are better understood by use of *in situ* diagnostics and characterization so that they can be controlled more precisely and dynamically. This research helps 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, is strengthened to take advantage of the opportunities to realize a more thorough understanding of these materials and their potential for bringing about transformational advances in energy and information technologies. Research on nanomaterials, traditional semiconductors, liquid crystals, and thin film transistor synthesis continues at a reduced level.	efficiency, including light weight polymers and interfacial chemistry, discovery of new classes of porous materials, and improved catalysts. Mastering nature's design rules such as hierarchical architecture and beyond-equilibrium matter to enable entirely new classes of functional materials will be a key challenge, as identified in the BES Advisory Committee report on transformative challenges for materials discovery. Research will include predictive models, including the incorporation of metastability, to guide the creation of beyond-equilibrium matter; synthesis and assembly of hierarchical structures for multi-dimensional hybrid matter; and in situ characterization of spatial and temporal evolution during synthesis and assembly. This effort will include harnessing coherence in light and matter, together with improving our understanding of the critical roles played by heterogeneity, interfaces and disorder.	materials during synthesis, in combination with computation and theory, to develop new predictive models of synthesis for targeted functionality that incorporate metastability and focus on non-equilibrium matter and assembly of hierarchical inorganic-organic hybrid materials. Other cross-cutting opportunities include exploring materials phenomena that transcend the nano-micro-meso scales, and underpin the processes at interfaces which are ubiquitous in nearly all energy technologies. The program will continue to deemphasize research on developing synthesis methods for nanomaterials, e.g., nanoparticles, nanorods, as well as maturing areas such as nanomaterial synthesis (not assembly), traditional semiconductors for solid-state lighting, thin film transistors, liquid crystals, and hydrogen storage materials for automotive applications.
Experimental Program to Stimulate Competitive Research (EPSCoR) $14,776,000	**$8,520,000**	**-$6,256,000**
Efforts continue to span science in support of the DOE mission, with continued emphasis on science that underpins DOE energy technology programs. Implementation grants, state-laboratory partnerships, and investment in early career research staff from EPSCoR states are sustained. Single investigator research that supports topics related to DOE mission areas, especially through the state-laboratory partnerships component of the program is emphasized.	Efforts will continue to span science in support of the DOE mission, with continued emphasis on science that underpins DOE energy technology programs. Implementation grants, state-laboratory partnerships, and investment in early career research staff from EPSCoR states will be sustained.	Research support is reduced compared to the FY 2016 Enacted level, returning the program to the requested funding levels. The FY 2017 program will focus on research topics identified by the Quadrennial Technology Review, the Department crosscuts, and the BES advisory committee report on transformative challenges for materials discovery.

FY 2016 Enacted	FY 2017 Request	Explanation of Changes FY 2017 vs FY 2016
Energy Frontier Research Centers (EFRCs) $55,800,000	**$55,800,000**	**$0**
The EFRCs continue to perform fundamental multi-disciplinary research aimed at accelerating scientific innovation. All EFRCs undergo a mid-term review in FY 2016 to assess progress toward meeting scientific research goals. DOE issues a Funding Opportunity Announcement for up to five new EFRC awards in FY 2016.	FY 2017 funds will provide the fourth year of funding for awards made in FY 2014, as well as the second year of funding for new awards made in FY 2016.	Research support is flat with the FY 2016 Enacted level.
Energy Innovation Hubs—Batteries and Energy Storage $24,137,000	**$24,088,000**	**-$49,000**
The Hub, in its fourth year, continues 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 completes 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.	In FY 2017, the last year of the first award period, the Hub will focus on developing energy storage research prototypes (components and cells) for transportation and grid applications that are based on beyond lithium ion concepts (e.g., multivalent ions, chemical transformation, non-aqueous redox flow), identified through JCESR research on materials discovery and techno-economic modeling. These prototypes will demonstrate the potential to scale-up to manufacturing prototype batteries that will meet the JCESR goal of delivering five times the energy density of 2011 battery systems at one-fifth the cost. Crosscutting fundamental research on materials characterization, theory, and modeling will continue to provide alternates for prototype development and to support JCESR's goals in 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.	The funding is approximately flat with the FY 2016 Enacted level, following the planned funding profile.
Computational Materials Sciences $12,000,000	**$12,000,000**	**$0**
Computational Materials Sciences advances U.S. leadership in the development of computational codes for materials sciences and engineering. The research	Basic research will continue to support the development of computational codes and the associated experimental and computational data to	The funding is flat compared to the FY 2016 Enacted level.

FY 2016 Enacted	FY 2017 Request	Explanation of Changes FY 2017 vs FY 2016
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 started in FY 2015 perform the first year of research as outlined in their proposals. This research focuses 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; the software will utilize current and future leadership class computers. Funding supports 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 is peer reviewed to assess management and early research activities.	provide predictive capability for design of functional materials. The research uses DOE user facilities to generate experimental data and synthesize materials to validate the predictions and DOE's leadership class computational capabilities in development of new software tools for materials discovery. In FY 2017, a mid-term peer review of the FY 2015 awards will assess the scientific progress of the individual activities, including progress towards the goal of providing open-source, community codes and publicly accessible databases.	

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 to develop a broad spectrum of new chemical processes, such as catalysis, that can contribute significantly to the advancement of new or cleaner 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 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 storage of carbon dioxide or waste products related to the energy sector.

- **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, with the goal of providing foundational knowledge of fundamental processes for energy capture, conversion, and storage.

The portfolio 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 systems, 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 and synthesis for the design of new catalytic methods and materials for clean and efficient production of fuels and chemicals. It also contains a unique effort in the fundamental chemistry of heavy elements, with complementary research on chemical separations and analysis. Crosscutting research of interfaces underpins a fundamental understanding of processes in catalysis, natural and artificial membranes, as well as geological systems. Research in geosciences emphasizes analytical and physical geochemistry especially in the subsurface, rock-fluid interactions, and flow/transport phenomena that are critical to a scientific understanding of geological storage of waste products such as carbon dioxide, produced water, or radioactive materials. 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 photo- and electrochemistry, photo-induced electron and energy transfer, and molecular assemblies for artificial photosynthesis. The subprogram also emphasizes the co-development of experimental and computational tools to continuously expand the complexity of research problems that can be investigated.

Among its efforts toward enabling advancement of clean energy technologies, the subprogram stresses research on efficient energy use and conversion and on chemistry in extreme environments. Highly efficient catalysts enable reduced energy use in industrial production and manufacturing, and photocatalysis can drive clean electricity generation and fuel production. New concepts, such as biomimetic approaches, are needed for design of efficient low-temperature catalysts and photocatalysts to enable clean energy conversion technologies. In extreme radiative environments, such as the natural decay of isotopes in nuclear waste, understanding of the complex dynamics and kinetics of heavy-element chemical processes is necessary for the design of remediating agents.

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. Use-inspired areas of research are emphasized with relevance, for example, to combustion and catalysis. The knowledge and techniques produced by this research form a science base that underpins numerous aspects of the DOE mission.

The principal research thrusts in this activity are atomic, molecular, and optical (AMO) sciences and chemical physics. AMO research emphasizes the interactions of atoms, molecules, and nanostructures with photons, particularly x-ray light, 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 goal is to develop accurate quantum mechanical descriptions of dynamical processes such as chemical bond breaking and forming, interactions in strong fields, and electron correlation.

Chemical physics research builds from the AMO foundation by examining the reactive chemistry of molecules whose chemistry is profoundly affected by the environment. The transition from molecular-scale chemistry to collective phenomena is explored in complex systems, such as the effects of solvation or interfaces on chemical structure and reactivity. Understanding such collective behavior is critical in a wide range of energy and environmental applications, from solar energy conversion to improved methods for including radiolytic effects in the context of advanced nuclear fuel or waste remediation. Gas-phase chemical physics emphasizes the rich and surprisingly complex 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 where accurate simulation of fundamental in-cylinder combustion/emission-formation processes and the effects of fuel composition will enable increased engine efficiency. 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. Computational and theoretical research supports the development and integration of new and existing theoretical and computational approaches for accurate and efficient descriptions of processes relevant to energy systems. Of special interest is foundational research on computational design of molecular- to meso-scale materials, and on next-generation simulation of complex dynamic processes.

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 efficient separation of reaction products and reacting phases, the chemistry of actinides important to nuclear energy, and the geological sequestration of waste products. 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, and lab and synchrotron techniques for in-situ characterization ranging from electrode surfaces to catalytic processes, with an emphasis on imaging chemically distinct species. This activity also supports training in radiochemistry and nuclear chemistry.

Theoretical and computational approaches are being developed to achieve a deeper understanding of reaction and separation processes, design new catalysts and membranes, and predict subsurface transport and reaction. 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 is likely to have broad impact in reducing manufacturing costs and energy consumption on a global scale.

This activity supports several research areas with potential impact on energy production, storage, and use. Advanced separation schemes for the removal of carbon dioxide from post-combustion streams are explored—these are essential to making carbon capture economical. Fundamental studies of the structure and reactivity of actinide-containing molecules provide the basis for their potential use in advanced nuclear energy systems. The extreme radiation environment involving radionuclides and the presence of elements containing f-electrons create complicated chemical systems exhibiting unique dynamic and kinetic behavior. The challenges are further compounded by the evolving chemical mixtures with time that must be understood to develop viable waste treatment options for the storage of nuclear waste and for the generation of clean nuclear energy. Geosciences improves understanding of the consequences of deliberate storage, or accidental discharge, of energy related products such as carbon dioxide, produced water or radioactive waste materials which requires ever more refined knowledge of how such species react and move in the subsurface environment. Subsurface fluid flow and complex chemistry occurring on a wide range of time scales are relevant not only for the efficient production of oil, gas, and geothermal energy but also for carbon sequestration and disposal of nuclear waste.

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. An important component of this activity is its leadership role in the support of basic research in both solar photochemistry and natural photosynthesis. A breadth of approaches and unique tools are developed and used to investigate the structural and chemical dynamics of energy absorption, transfer, conversion and storage across spatial and temporal scales. The fundamental chemical and physical concepts from the study of both natural systems (e.g. photosynthetic and affiliated downstream biological processes) and man-made chemical systems provide crucial foundational knowledge for using solar energy and photocatalysis to drive clean electricity generation and fuel production and for developing efficient, environmentally benign, sustainable catalysts that can help enable next generation clean energy conversion technologies.

Natural photosynthesis is studied to understand the dynamic mechanisms of solar energy capture and conversion in biological systems and to provide roadmaps for the creation of robust artificial and bio-hybrid systems that exhibit 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 chemical and artificial systems encompasses organic and inorganic photochemistry, electrochemistry, light-driven energy and electron transfer processes, and molecular assemblies for electricity generation and artificial photosynthetic fuel production. Fundamental knowledge resulting from these studies of complex chemical processes and electron dynamics under changing environmental conditions can provide an important foundation for the development of efficient solar energy technologies.

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 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. The current 32 centers (22 of which were renewed from the initial group, and 10 of which are new centers initiated in FY 2014) continue to expand upon these accomplishments. These EFRCs are 4-year awards with funding for the final two years contingent upon the successful outcome of a mid-term review.

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.

In response to two strategic planning activities related to the Subsurface crosscut, additional funds are requested in FY 2017 to fully support up to five new EFRC awards to address the grand challenge of "Advanced imaging of geophysical and geochemical signals in the subsurface." The scientific focus will be on fracture networks, associated fluid flow and reaction, and the gaps in fidelity, resolution, and conceptual understanding of subsurface imaging in hard-to-access environments. Current limitations to fully exploiting our subsurface energy resources in an environmentally responsible manner lie in the inadequate resolution attainable in seismic imaging, in traditional sampling techniques before and after injection that provide insufficient insight into fluid elements and isotopic composition over extended length and time scales, and in the effect of physical changes and concurrent geochemical processes in rock-fluid systems associated with subsurface and geological engineering.

The EFRC model has proven effective in promoting partnerships and addressing grand challenge science requiring multidisciplinary teams focused on discrete problems with novel approaches. Efforts will build on cross-cutting themes such as advanced, predictive computational methods to describe heterogeneous time-dependent studies of geologic systems; new laboratory studies on both natural and geo-architected subsurface materials that deploy advanced high-resolution 3D imaging; and chemical analysis methods to determine the rates and mechanisms of fluid-rock processes. The EFRC R&D platforms will be closely coupled with field-based approaches to enable the translation of scientific knowledge to practical solutions in subsurface engineering. A key deliverable will be the development of experimental imaging tools and computational approaches broadly applicable to the field of subsurface science.

<u>Energy Innovation Hubs—Fuels from Sunlight</u>
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 and eliminating waste streams from fossil fuel production, such as produced water, and from fossil fuel use, such as CO_2.

Due to the significant scientific and engineering challenges associated with developing such a system, however, there are no commercially-available fuels generated via artificial photosynthesis. For this reason, the Basic Energy Sciences Advisory

Committee report, New Science for Secure and Sustainable Energy Future,[a] listed the production of fuels directly from sunlight as one of three strategic goals for which transformational science breakthroughs are most urgently needed.

Established in September 2010, the Fuels from Sunlight Hub, 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. 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.

JCAP's efforts are synergistically split between JCAP-South on the campus of Caltech and JCAP-North located at LBNL, with the exception of the benchmarking and high-throughput experimentation projects that are consolidated at JCAP-South. JCAP makes use of state-of-the-art facilities at LBNL and SLAC as part of its efforts to examine, understand, and manipulate matter at the nanoscale. Despite the different geographic locations, JCAP operates as a single scientific entity. Its 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 initial award for the Fuels from Sunlight Hub ended on September 29, 2015. During this award period, research at JCAP centered primarily on the production of hydrogen fuel with smaller efforts addressing the considerably more challenging area of carbon-based fuels. Selected accomplishments during the first award term include discovery of new mechanisms and materials for electrocatalytically splitting water, identification of a novel oxygen evolution reaction catalyst, establishment of objective standardized procedures for evaluation of the efficacy and stability of electrocatalysts, and development of a semiconductor protection method capable of expanding the range of materials that can be used in solar fuel generators. Most importantly, JCAP reached its five-year goal to design and develop a photocatalytic prototype capable of generating fuel, specifically hydrogen, from sunlight. In December 2014, BES solicited a renewal proposal from JCAP for a final award term with a maximum duration of five years and directed JCAP to focus on the fundamental science of carbon dioxide reduction, a critical need for efficient solar-driven production of carbon-based liquid transportation fuels.

Based on the outcome of external peer review, the Fuels from Sunlight Hub was renewed by BES for a final five-year award term starting on September 30, 2015, at an annual funding level of $15M. The renewal leverages accomplishments and infrastructure from the initial award and maintains the unified operation led by Caltech in primary partnership with LBNL. SLAC National Accelerator Laboratory, the University of California, Irvine, and the University of California, San Diego, also remain as partners in the Hub. The objectives of the renewal project include the discovery and understanding of highly selective catalytic mechanisms for carbon dioxide reduction and oxygen evolution operating under defined conditions; accelerated discovery of electrocatalytic and photoelectrocatalytic materials and light-absorber photoelectrodes for selective and efficient carbon dioxide reduction into hydrocarbon fuels; and, using JCAP prototypes, demonstration of highly efficient and selective artificial photosynthetic carbon dioxide reduction and oxygen evolution components.

Computational Chemical Sciences

Computational Chemical Sciences is a new activity in FY 2017 to develop open-source modular software tools that can be reused as plug-and-compute tools for the basic energy sciences community in preparation for the arrival of exascale computing facilities and for the optimized usage of existing petascale computers, leveraging the U.S.' leadership in the development of computational chemistry codes.

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[a] 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.

Software solutions and infrastructure as enabling tools are necessary components of an effective scientific strategy to address the nation's energy challenges. Codes such as GAUSSIAN, GAMESS and NWChem have established U.S. dominance in computational chemistry; that leadership is now being challenged with the transition to predominantly massively-parallel high performance computing platforms. Today's best chemical simulation codes are currently unable to efficiently use more than one percent of the processors available on existing leadership-class supercomputers. A systematic effort to modify or replace existing computational chemistry codes with codes that are well-adapted to anticipated exascale architectures is critically needed.

Recent breakthroughs in computational chemistry provide a strong foundation for future success in this activity. For example, researchers developed a density-functional based predictive method with unprecedented accuracy for gas phase thermochemistry. This method is based upon a new and systematically improvable genomic framework and, for the first time, delivers energetics that rival those of the most-accurate wavefunction-based computational chemistry codes. Unlike the latter, the new predictive paradigm can in principle be extended to methods that are amenable to atoms in the lower half of the periodic table, and to structures composed of a solid-gas/liquid interface which are particularly important to the chemistry-based energy sciences. Such systems form the molecular building blocks for catalysts, gas-separation technologies, and natural and artificial photosynthesis.

In this activity, computational chemists will deploy these capabilities in all major open-source chemical simulation-software used by the community, rewrite software and algorithms to fully realize the current and future gains in efficiency offered by massively parallel computing platforms and systematically alleviate the need to employ semi-empirical case-by-case corrections. Tackling these enormously complex challenges will require multi-investigator teams to combine theoretical, computational and algorithmic advances to jointly increase by at least 1,000 times the accuracy and speed of molecular and chemical design.

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.

Activities and Explanation of Changes

FY 2016 Enacted	FY 2017 Request	Explanation of Changes FY 2017 vs FY 2016
Chemical Sciences, Geosciences, and Biosciences $312,061,000	**$387,356,000**	**+$75,295,000**
Fundamental Interactions Research $74,599,000	**$79,233,000**	**+$4,634,000**
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, to probe and control atomic, molecular, nanoscale and mesoscale matter. The program continues to develop advanced theoretical methods to guide and interpret ultrafast measurements and to design new experiments. It also continues to emphasize time-resolved electron and x-ray probes of matter at unprecedented short time scales and in systems of increasing complexity. Computational efforts stress the development of improved methods to calculate electronically excited states in molecules and extended mesoscale systems. Work continues on advanced combustion research to accelerate the predictive simulation of highly efficient and clean internal combustion engines. Increased emphasis is on investigating properties of combustion in high-pressure or multiphase systems. The program deemphasizes research at the interface of nanoscience with molecular physics.	Research will continue to develop and apply forefront ultrafast x-ray and optical probes of matter using the LCLS, BES synchrotron light sources, and table-top laser-based ultrafast light sources to probe and control atomic, molecular, nanoscale and mesoscale matter. The program will continue to develop advanced theoretical methods to guide and interpret ultrafast measurements and to design new experiments. It will also continue to emphasize the development of novel instrumentation for time-resolved electron and x-ray probes of matter at ultrafast 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 to characterize and model chemical systems. Work will continue on advanced combustion research to accelerate the predictive simulation of highly efficient and clean internal combustion engines. The program will place Increased emphasis on investigating properties of combustion in high-pressure or multiphase systems.	Research support increases compared to the FY 2016 Enacted level to include a new multidisciplinary effort in energy efficiency with the goal to develop operating conditions compatible with new catalysts and renewable fuels in combustion engines. To maintain support for forefront research in ultrafast science, the FY 2017 program deemphasizes research on ultra-cold molecules and molecular and particle spectroscopy. The program also supports investments in predictive theory and modeling to guide and interpret increasingly complex measurements of chemical processes in preparation for the arrival of exascale computing capabilities through the proposed Computational Chemical Sciences program.
Chemical Transformations Research $92,341,000	**$106,423,000**	**+$14,082,000**
Synthesis, guided by theory and computation, continues 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 program emphasizes catalytic conversion of biomass to fuels and other energy related chemical products as well as the search	Guided by theory and computation, the research will continue to design and synthesize novel catalytic materials at the nano- and mesoscale for the efficient conversion of traditional and new feedstocks into higher-value fuels and other chemicals, with a new emphasis on energy efficiency. The program will continue to emphasize the catalytic conversion of	The funding increase will enhance this program's contribution to the Subsurface crosscut with an emphasis on fundamental geochemistry and geophysics, specifically subsurface fluid flow and complex chemistry on timescales of microseconds to millennia with importance for oil and gas production, geothermal energy, carbon capture and storage, and

FY 2016 Enacted	FY 2017 Request	Explanation of Changes FY 2017 vs FY 2016
for catalysts for new ammonia production routes that avoid the generation of greenhouse gases. To support these new emphases, the program will deemphasize the development of mass spectrometric techniques. Likewise, coupled predictive theory and synthesis of designer mesoporous membranes and filter materials seek more efficient separation of carbon dioxide from power plant effluents or of oxygen from air relevant to oxycombustion approaches. Subsurface geochemistry and geophysics 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 continues 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 continues in parallel with efforts in other offices as coordinated by the Subsurface Science, Technology and Engineering R&D (Subsurface) crosscut.	biomass and light alkanes to fuels and other energy related chemical products. Likewise, coupled predictive theory and synthesis of designer mesoporous membranes and filter materials will continue to seek more efficient separation of carbon dioxide and environmentally malign products of combustion from conventional or advanced power plants. Subsurface geochemistry and geophysics will seek to provide data and mechanistic interpretation for models of reactive flow and transport important for waste 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 fuel and waste processes, particularly using ionic liquids. Fundamental research activities in geochemistry and geophysics of the subsurface will continue in FY 2017 in parallel with efforts in other offices as coordinated by the Subsurface crosscut.	nuclear waste disposal. In addition, the increase will support new directions in energy efficiency and chemistry in extreme environments. The program will target new catalysts capable of operating at low temperatures and inspired by natural systems, as well as synergistic approaches such as electro- and photoelectrocatalysis. This research is a cross disciplinary effort between the Chemical Transformations and the Photochemistry and Biochemistry Research areas. Chemistry research in extreme environments focuses on elucidating the nature, dynamics, and kinetics of complex chemical processes in the highly radiative nuclear waste environment. Understanding such processes is further complicated by the involvement of f-electrons for heavy elements. Research in this area will focus on the bonding, chemical reactivity, and the design of selective agents to extract unwanted species from the waste mixture. Investments in mass spectrometric tools will be deemphasized since it has reached a high level of technical maturity.
Photochemistry and Biochemistry Research		
$64,189,000	**$71,197,000**	**+$7,008,000**
Research continues 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. The program continues to support efforts in computation and modeling 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. The program continues to emphasize research to	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. The program will continue to support efforts in computation and modeling 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. Continued work in electrochemistry and	Research support is increased compared to the FY 2016 Enacted level to include a new multidisciplinary effort in energy efficiency and chemistry in extreme environments. This research is part of a synergistic cross-disciplinary effort between the Photochemistry and Biochemistry Research and Chemical Transformations Research areas to establish energy efficient catalysts and understand chemical dynamics during energy conversion and in radiative environments, building on the expertise in radiation chemistry, photo(electro) catalysis, and enzyme-mediated (biological) catalysis. Such research can span

FY 2016 Enacted	FY 2017 Request	Explanation of Changes FY 2017 vs FY 2016
understand the fundamental mechanisms of water-splitting, redox, cell wall biosynthesis, and other energy-relevant biological (enzymatic) reactions, from the nano- to the mesoscale. These studies 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. The program deemphasizes research on fundamental mechanisms of carbon capture.	photocatalysis will seek to advance development of solar energy conversion for generation of electricity and chemical fuels, as will research to identify and characterize potential new mechanisms, such as perovskites, to increase efficiency of solar energy conversion and use. The program will continue to emphasize research to understand the fundamental mechanisms of water-splitting, redox, dynamical complex assembly, electron and other energy-relevant biological (enzymatic) reactions, from the nano- to the mesoscale. These studies will provide 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.	different time and spatial scales, for instance from understanding electron dynamics to determining mechanisms important for efficient complex assembly and function. The program will deemphasize efforts in the study of plant hormones, biotic stress and on the development of genetic systems to allow investments in the basic research of dye-sensitized solar cells and the analysis of the structure, function, and mechanism of enzymes that mediate the flow of electrons in biological systems.
Energy Frontier Research Centers (EFRCs) $54,200,000	**$86,766,000**	**+$32,566,000**
The EFRCs continue to perform fundamental multi-disciplinary research aimed at accelerating scientific innovation. All EFRCs undergo a mid-term review in FY 2016 to assess progress toward meeting scientific research goals. DOE issues a Funding Opportunity Announcement for up to five new EFRC awards in FY 2016.	FY 2017 funds will provide the fourth year of funding for awards made in FY 2014 as well as the second year of funding for new awards made in FY 2016. New funds in FY 2017 will fully support up to five new EFRCs related to the Subsurface crosscut to develop experimental imaging tools and computational approaches broadly applicable to the field of subsurface science.	The funding increase will enhance the BES contribution to the Subsurface crosscut by addressing the grand challenge "Advanced imaging of geophysical and geochemical signals in the subsurface," with a focus on fracture networks, associated fluid flow and reaction, and the gaps in fidelity, resolution, and conceptual understanding of subsurface imaging in hard-to-access environments. Funds are requested to enable up to five new awards for multidisciplinary teams from DOE laboratories, industry, and academia to work closely with field-based projects to address the grand challenge identified in the 2015 Subsurface strategic planning workshops.
Energy Innovation Hubs—Fuels From Sunlight $15,000,000	**$15,000,000**	**$0**
The Fuels from Sunlight Hub was renewed for a final award term of up to 5 years starting in September 2015. Research in the renewal focuses on the fundamental science needed to enable efficient,	The Fuels from Sunlight Hub will continue to perform research on the fundamental science of carbon dioxide reduction needed to enable efficient, sustainable solar-driven production of liquid transportation fuels.	Research support is flat with the FY 2016 Enacted level.

FY 2016 Enacted	FY 2017 Request	Explanation of Changes FY 2017 vs FY 2016
sustainable and scalable photochemical reduction of carbon dioxide for production of liquid transportation fuels. The renewal allows JCAP to further advance research efforts addressing critical needs in solar fuels development and to capitalize on its achievements and infrastructure development from the initial funding period. JCAP undergoes a scientific and merit review in FY 2016 to assess progress toward meeting project milestones and goals.	JCAP will undergo a scientific and merit review in FY 2017 to assess progress toward meeting project milestones and goals.	
Computational Chemical Sciences $0	**$13,635,000**	**+$13,635,000**
N/A	A new investment in Computational Chemical Sciences will develop open-source modular software tools that can be reused and tailored for the specific needs of the basic research community, essentially acting as "plug-and-compute" tools. While the U.S. is a leader in the development of computational chemistry codes such as GAUSSIAN, GAMESS, and NWChem, U.S. leadership is being challenged with the transition to predominantly massively-parallel computer platforms. The best chemical simulation codes are currently unable to efficiently use more than one percent of the processors available on existing leadership computers. A systematic effort to modify or replace existing computational chemistry codes with codes that are well-adapted to anticipated exascale architectures is critically needed. This investment will build on current quantum chemistry software, seeking to create new codes that fully leverage massively-parallel high performance computing platforms.	This new activity readies the computational chemistry community for the arrival of exascale computer systems and optimizes the use of current petascale capabilities of DOE's Leadership Computing Facilities as an enabling tool for the development of new quantum chemical codes to predict, model and solve complex chemical problems. BES will start extending the quantum chemistry codes to other systems, including processes in molecular complexes composed of atoms in the lower two-thirds of the periodic table (i.e., belonging to the d- and f-block elements). Topical areas of emphasis will also include membranes and structures composed of a solid-gas/liquid interface. Advances in these areas are particularly important to the chemistry-based energy sciences, as such systems form the molecular building blocks for catalysts, gas-separation technologies, and natural and artificial photosynthesis.
General Plant Projects $1,000,000	**$1,000,000**	**$0**
Funding supports minor facility improvements at Ames Laboratory.	Funding will support minor facility improvements at Ames Laboratory.	Funding is flat with the FY 2016 Enacted level.

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 with wavelengths at least as small as the structures being investigated. The BES 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.

In FY 2015, the BES scientific facilities were used by more than 14,000 scientists and engineers in many fields of science and technology. These facilities provide unique capabilities to the scientific community and industry 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 at no cost to researchers who intend to publish their results in the open literature.

<u>Synchrotron Radiation Light Sources</u>
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.

<u>High Flux Neutron Sources</u>
One of the goals of modern materials science is to understand the factors that determine the properties of matter on the atomic scale and to use this knowledge to optimize those properties or to develop new materials and functionality. This process regularly involves the discovery of fascinating new physics, which itself may lead to previously unexpected applications. Among the different probes used to investigate atomic-scale structure and dynamics, 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 12 instruments in the user program at HFIR and the adjacent cold neutron beam guide hall, which 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. 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.

<u>Nanoscale Science Research Centers (NSRCs)</u>
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 not

found in nature, and observe and understand how they function and 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. They are a different class of facility than the x-ray and neutron sources, as NSRCs are not based on a large accelerator or reactor but are comprised of a suite of smaller unique tools and expert scientific staff. 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 nanomaterials synthesis and assembly; theory, modeling and simulation; imaging and spectroscopy including electron microscopy; and nanostructure fabrication and 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, electron scattering, or computation 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. The NSRC electron microscopy capabilities provide superior atomic-scale spatial resolution and the ability to simultaneously obtain structural, chemical, and other types of information from sub-nanometer regions at short time scales. 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 academic, government, and industry researchers with access determined through external peer review of user proposals.

<u>Other Project Costs</u>

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.

<u>Major Items of Equipment</u>

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.

<u>Research</u>

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 development of intense laser-based THz sources to study non-equilibrium behavior in complex materials. 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. X-ray optics research involves development of systems for time-resolved x-ray science that preserve the spatial, temporal, and spectral properties of x-rays. 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 training in the field of particle beams and their associated accelerator technologies.

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.

Activities and Explanation of Changes

FY 2016 Enacted	FY 2017 Request	Explanation of Changes FY 2017 vs FY 2016
Scientific User Facilities $966,849,000	**$963,529,000**	**-$3,320,000**
Synchrotron Radiation Light Sources $481,906,000	**$489,059,000**	**+$7,153,000**
Funding supports 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 provided for NSLS as it ceased operations in FY 2015. $5M is for R&D in support of the Advanced Light Source Upgrade.	The FY 2017 Request includes funding for optimal operations of the five BES light sources to fully support research, including clean energy research. These five operating facilities together are responsible for almost 75% of the total users of BES national user facilities. It is essential that these facilities be fully staffed and that funding be provided for high-priority upgrades of beam lines and other equipment essential for the users' research. The request also includes funds to expand the beamline capabilities for the newly constructed NSLS-II and to enhance the ability of users to perform cutting-edge research at the only free electron laser x-ray source in the U.S.	The funding increase will support optimal operations and allow the facilities to proceed with necessary maintenance, routine accelerator and instrumentation improvements, and crucial staff hires or replacements. The request will support the development of beamlines for the newly constructed NSLS-II based on reconfigured equipment from NSLS that will make use of the high brightness available at NSLS-II.
High-Flux Neutron Sources $264,645,000	**$261,177,000**	**-$3,468,000**
Funding supports the operation of HFIR and SNS at near optimal levels. Limited funding is included for the Lujan Neutron Scattering Center for the removal of hazardous materials and planning of the disposition of unused equipment. $10M is provided to accelerate the progress towards critical decision-1 for the Second Target Station at SNS.	The FY 2017 Request includes funding for optimal operation of HFIR and SNS at Oak Ridge National Laboratory (ORNL) to fully support research, including clean energy research. Part of this funding supports selected strategic hires at the neutron facilities to enhance the overall scientific impact and breadth of the facility research program and to increase collaborative programs with the ORNL Center for Nanophase Materials Science. The funding will allow purchase and installation of additional detectors on selected instruments at the SNS to increase their overall productivity and will also fund other critically needed high priority instrument enhancements. At HFIR, the FY 2017 Request also funds critical upgrades to older triple axis spectrometers to improve resolution and data collection efficiency. The request	The funding increase will support optimal operations and necessary maintenance of the neutron sources, high priority upgrades to instruments, and crucial staff hires or replacements.

FY 2016 Enacted	FY 2017 Request	Explanation of Changes FY 2017 vs FY 2016
	also includes funds for planning and initial disposition of unused equipment at the Lujan Center.	
Nanoscale Science Research Centers $118,763,000	**$122,272,000**	**+$3,509,000**
Funding supports operations at the NSRCs at near optimal levels. Program emphasis continues to cultivate and expand the user base from universities, national laboratories, and industry. Planning efforts 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 Request includes funding for optimal operations of the five Nanoscale Science Research Centers to fully support research, including clean energy research. Funding will be used to exploit synergies between the NSRCs and major co-located x-ray, neutron, computation and fabrication facilities including developing new beamlines. These efforts build tools and capabilities to address challenges in characterizing ultrafast chemical and physical nanoscale phenomena in real environments. Joint activities involving all NSRCs such as workshops will be continued.	The funding increase will support optimal operations and instrument repairs, and replacement. Some NSRCs will begin developing joint capabilities with their co-located facilities.
Other Project Costs $0	**$0**	**$0**
No funds are requested for Other Project Costs.	No funds are requested for Other Project Costs.	No funds are requested.
Major Items of Equipment $35,500,000	**$20,000,000**	**-$15,500,000**
The Advanced Photon Source-Upgrade (APS-U) project continues 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 will continue activity associated with R&D, engineering design, equipment prototyping and equipment fabrication in preparation for long lead procurements in FY 2017.	The FY 2017 Request for APS-U is flat compared to the FY 2016 Enacted level.
The NSLS-II Experimental Tools (NEXT) project continues with the design, procurements, construction/fabrication, installation, testing and commissioning of equipment during FY 2016.	No funds are requested for NEXT in FY 2017. NEXT will continue with the remaining design, procurements, construction/fabrication, installation, testing and commissioning of equipment during FY 2017. The project will complete by the end of FY 2017.	FY 2016 is the last year of funding for NEXT per the project plan.

FY 2016 Enacted	FY 2017 Request	Explanation of Changes FY 2017 vs FY 2016
Research $34,853,000	**$37,537,000**	**+$2,684,000**
The research funding for the scientific user facilities continues to support selected, high-priority research activities. This funding supports activities to ensure that the scientific user facilities continue to demonstrate performance excellence, with focused efforts to address next generation facilities research needs. Emphasis is 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 included.	The FY 2017 Request will allow concerted efforts in innovative concepts in beam acceleration techniques and expanded development of advanced instrumentation for beam characterization, measurement, and control to enable the full utilization of the high flux, brilliance, and ultra-short pulses provided by the new light sources, and increased intensity at the neutron sources. As part of the Presidential BRAIN Initiative and in close coordination with the National Institutes of Health (NIH), BES will develop next generation tools and technologies at DOE X-ray Light Sources and Nanoscale Science Research Centers to enable advances in brain imaging and sensing. The research will focus on developing novel tools and bio-compatible nano-materials to improve the sensitivity and the spatial and temporal resolution of imaging and sensing of neural transmission, and on developing bio-compatible nanomaterials for studying these systems with potential for use in medicine. Funding to continue the long term surveillance and maintenance responsibilities at BNL and SLAC is included.	The increase supports development of tools and technologies related to the Presidential BRAIN Initiative as well as novel methods of beam acceleration and additional development of instruments and techniques to measure and control particle and photon beams. Funding for long term surveillance and maintenance is reduced according to project needs.

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.

In April 2015, the Office of Science conducted an external Independent Project Review (IPR) to assess the project's readiness for Critical Decision-3B (CD-3B), Approve Long Lead Procurements. Based on the positive IPR review outcome, the CD-3B was approved on May 28, 2015 which authorized long lead and advanced procurements for key components of the cryoplant and the superconducting linac which are on the critical path for the project. The IPR committee also recommended increasing the cryoplant refrigeration capacity to mitigate technical risks. The recommendation was accepted by BES and the project and led to an increase of the preliminary total project cost (TPC) point estimate from $965,000,000 to $1,045,000,000.

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 best practices in project management. In accordance with DOE Order 413.3B, each project is closely monitored and must perform within 10% of the cost and schedule performance baselines, established at Critical Decision 2, Approve Performance Baseline, and which are reproduced in the construction project data sheet.

Activities and Explanation of Changes

FY 2016 Enacted	FY 2017 Request	Explanation of Changes FY 2017 vs FY 2016
Construction $200,300,000	**$190,000,000**	**-$10,300,000**
Linac Coherent Light Source-II (LCLS-II) $200,300,000	**$190,000,000**	**-$10,300,000**
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 fabricates technical equipment during FY 2016.	The FY 2017 Request supports the continuation of the construction effort according to the project plan.	The FY 2017 Request decreases compared to the FY 2016 Enacted level.

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. The following table shows the targets for FY 2015 through FY 2017. Details on the Annual Performance Report can be found at http://energy.gov/cfo/reports/annual-performance-reports.

	FY 2015	FY 2016	FY 2017
Performance Goal (Measure)	**BES Facility Operations—Average achieved operation time of BES user facilities as a percentage of total scheduled annual operation time**		
Target	≥ 90%	≥ 90%	≥ 90%
Result	Met	TBD	TBD
Endpoint Target	Many of the research projects that are undertaken at the Office of Science's scientific user facilities take a great deal of time, money, and effort to prepare and regularly have a very short window of opportunity to run. If the facility is not operating as expected, the experiment could be ruined or critically set back. In addition, taxpayers have invested millions or even hundreds of millions of dollars in these facilities. The greater the period of reliable operations, the greater the return on the taxpayers' investment.		
Performance Goal (Measure)	**BES Facility Construction/MIE Cost & Schedule—Cost-weighted mean percent variance from established cost and schedule baselines for major construction, upgrade, or equipment procurement projects.**		
Target	< 10%	< 10%	< 10%
Result	Met	TBD	TBD
Endpoint Target	Adhering to the cost and schedule baselines for a complex, large scale, science project is critical to meeting the scientific requirements for the project and for being good stewards of the taxpayers' investment in the project.		
Performance Goal (Measure)	**BES Energy Storage—Deliver two high-performance research energy storage prototypes for transportation and the grid that project at the battery pack level to be five times the energy density at 1/5 the cost of the 2011 commercial baseline.**		
Target	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.	Develop and demonstrate energy storage research prototypes that are scalable for transportation and grid applications using concepts beyond lithium ion (multivalent ions, chemical transformation, and non-aqueous redox flow), as identified through materials discovery and techno-economic modeling.
Result	Met	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 *Batteries and Energy Storage* Energy Innovation Hub.		

Basic Energy Science
Capital Summary ($K)

	Total	Prior Years	FY 2015 Enacted	FY 2015 Current	FY 2016 Enacted	FY 2017 Request	FY 2017 vs FY 2016
Capital Operating Expenses Summary							
Capital Equipment	n/a	n/a	48,100	67,105	41,000	29,500	-11,500
General Plant Projects (GPP)	n/a	n/a	600	1,800	1,000	1,000	0
Accelerator Improvement Projects (AIP)	n/a	n/a	9,925	5,150	9,425	13,000	+3,575
Total, Capital Operating Expenses	**n/a**	**n/a**	**58,625**	**74,055**	**51,425**	**43,500**	**-7,925**
Capital Equipment							
Major Items of Equipment							
Advanced Photon Source Upgrade (APS-U), ANL (TPC TBD)[a]	TBD	68,500	20,000	20,000	20,000	20,000	0
Linac Coherent Light Source-II (LCLS-II), SLAC[b,c]	—	85,600	0	0	0	0	0
NSLS-II Experimental Tools (NEXT), BNL (TPC $90,000)	90,000	52,000	22,500	22,500	15,500	0	-15,500
Total, Major Items of Equipment	n/a	n/a	42,500	42,500	35,500	20,000	-15,500
Total, Non-MIE Capital Equipment	n/a	n/a	5,600	24,605	5,500	9,500	+4,000
Total, Capital equipment	**n/a**	**n/a**	**48,100**	**67,105**	**41,000**	**29,500**	**-11,500**
General Plant Projects (GPP)							
Other general plant projects under $5 million TEC	n/a	n/a	600	1,800	1,000	1,000	0
Accelerator Improvement Projects (AIP)							
Accelerator improvement projects under $5 million TEC	n/a	n/a	9,925	5,150	9,425	13,000	+3,575

[a] Following the July 2013 BESAC report on Future X-Ray Light Sources, the APS-U project has been rescoped to upgrade to a fourth generation storage ring and beamlines.
[b] LCLS-II is requested as a line item construction project beginning in FY 2014.
[c] 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 develop, design, build, install, and test the equipment necessary to upgrade an existing third-generation synchrotron light source facility, the Advanced Photon Source (APS). The FY 2017 Request for the APS-U is $20,000,000, which is flat compared to the FY 2016 Enacted level. The APS is one of the Nation's most productive x-ray light source facilities, serving over 5,000 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 one of only four in the world, along with the European Synchrotron Radiation Facility (ESRF) in France, PETRA-III in Germany, and SPring-8 in Japan. In 2015 China announced its intention to construct a fourth generation 6 GeV hard x-ray synchrotron light source. High-energy penetrating x-rays are 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 21st Century. In response to the findings and recommendations of the July 25, 2013 BES Advisory Committee report, the APS-U Project will upgrade the existing APS to provide scientists with an x-ray source possessing world-leading transverse coherence and extreme brightness. The magnetic lattice of the APS storage ring will be upgraded to a multi-bend achromat configuration to provide 100-1000 times increased brightness and coherent flux. The APS-U 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.

The National Synchrotron Light Source-II (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. FY 2016 is the last year of construction funding for NEXT; no funding is requested in FY 2017. The NEXT Project will provide NSLS-II with complementary best-in-class beamlines that support the identified needs of the U.S. research community and the DOE energy mission. Implementation of this state-of-the-art instrumentation will significantly increase the scientific quality and productivity of NSLS-II. In addition, the NEXT project will enable and enhance more efficient operation of NSLS-II. The project is managed by Brookhaven National Laboratory.

Construction Projects Summary ($K)

	Total	Prior Years	FY 2015 Enacted	FY 2015 Current	FY 2016 Enacted	FY 2017 Request	FY 2017 vs FY 2016
13-SC-10, Linac Coherent Light Source-II (LCLS-II), SLAC							
TEC	993,100	142,700	138,700	138,700	200,300	190,000	-10,300
OPC	51,900	28,600	9,300	9,300	0	0	0
TPC	**1,045,000**	**171,300**[a]	**148,000**	**148,000**	**200,300**	**190,000**	**-10,300**
Total, Construction							
TEC	n/a	n/a	138,700	138,700	200,300	190,000	-10,300
OPC	n/a	n/a	9,300	9,300	0	0	0
TPC	**n/a**	**n/a**	**148,000**	**148,000**	**200,300**	**190,000**	**-10,300**

Funding Summary ($K)

	FY 2015 Enacted	FY 2015 Current	FY 2016 Enacted	FY 2017 Request	FY 2017 vs FY 2016
Research	686,876	681,346	692,214	791,188	+98,974
Scientific User Facilities Operations	804,948	810,078	865,314	872,508	+7,194
Major Items of Equipment	42,500	42,500	35,500	20,000	-15,500
Construction Projects (includes OPC)	148,000	148,000	200,300	190,000	-10,300
Other[b]	50,876	1,000	55,672	63,034	+7,362
Total, Basic Energy Sciences	**1,733,200**	**1,682,924**	**1,849,000**	**1,936,730**	**+87,730**

[a] LCLS-II received $85,600,000 in FY 2010-FY 2013 as an MIE.
[b] 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 2015 Enacted	FY 2015 Current	FY 2016 Enacted	FY 2017 Request	FY 2017 vs FY 2016
TYPE A FACILITIES					
Advanced Light Source	**$60,500**	**$61,250**	**$68,050**	**$64,950**	**-$3,100**
Number of Users	2,400	2,560	2,450	2,400	-50
Achieved operating hours	N/A	5,770	N/A	N/A	N/A
Planned operating hours	5,000	5,000	5,200	5,000	-200
Optimal hours	5,300	5,300	5,300	5,000[a]	-300
Percent optimal hours	94.3%	108.9%	98.1%	100%	N/A
Unscheduled downtime hours	<10%	<10%	<10%	<10%	N/A

[a] Optimal hours decreased for scheduled maintenance.

	FY 2015 Enacted	FY 2015 Current	FY 2016 Enacted	FY 2017 Request	FY 2017 vs FY 2016
Advanced Photon Source	**$124,815**	**$125,540**	**$130,432**	**$133,995**	**+$3,563**
Number of Users	5,000	5,331	5,100	5,000	-100
Achieved operating hours	N/A	4,944	N/A	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	100%	98.9%	100%	100%	N/A
Unscheduled downtime hours	<10%	<10%	<10%	<10%	N/A
National Synchrotron Light Source, BNL	**$5,500**	**$7,000**	**$0**	**$0**	**$0**
Achieved operating hours	N/A	N/A	N/A	N/A	N/A
Planned operating hours	0	0	0	0	0
Optimal hours	0	0	0	0	0
Percent optimal hours	N/A	N/A	N/A	N/A	N/A
Unscheduled downtime hours	N/A	N/A	N/A	N/A	N/A
National Synchrotron Light Source-II, BNL	**$90,415**	**$90,715**	**$110,000**	**$111,834**	**+$1,834**
Number of Users	200	110	700	900	+200
Achieved operating hours	N/A	1,965	N/A	N/A	N/A
Planned operating hours	2,100	2,100	3,250	3,500	+250
Optimal hours	2,300	2,300	3,300	3,500	+200
Percent optimal hours	91.3%	85.4%	98.5%	100%	N/A
Unscheduled downtime hours	<10%	<10%	N/A	<10%	N/A
Stanford Synchrotron Radiation Lightsource	**$39,000**	**$39,798**	**$40,755**	**$41,986**	**+$1,231**
Number of Users	1,500	1,626	1,550	1,500	-50
Achieved operating hours	N/A	4,925	N/A	N/A	N/A
Planned operating hours	5,200	5,200	5,300	5,200	-100
Optimal hours	5,400	5,400	5,400	5,200[a]	-200
Percent optimal hours	96.3%	91.2%	98.1%	100%	N/A
Unscheduled downtime hours	<10%	<10%	<10%	<10%	N/A

[a] Optimal hours decreased for scheduled maintenance.

	FY 2015 Enacted	FY 2015 Current	FY 2016 Enacted	FY 2017 Request	FY 2017 vs FY 2016
Linac Coherent Light Source	**$126,956**	**$125,800**	**$132,669**	**$136,294**	**+$3,625**
Number of Users	580	837	580	380	-200
Achieved operating hours	N/A	4,555	N/A	N/A	N/A
Planned operating hours	4,700	4,700	4,600	3,000	-1,600
Optimal hours	4,700	4,700	4,700	3,000[a]	-1,700
Percent optimal hours	100%	96.9%	97.9%	100%	N/A
Unscheduled downtime hours	<10%	<10%	<10%	<10%	N/A
High Flux Isotope Reactor	**$60,688**	**$61,625**	**$63,419**	**$64,968**	**+$1,549**
Number of Users	450	491	450	450	0
Achieved operating hours	N/A	3,658	N/A	N/A	N/A
Planned operating hours	3,400	3,400	3,450	3,500	+50
Optimal hours	3,500	3,500	3,500	3,500	0
Percent optimal hours	97.1%	104.5%	98.6%	100%	N/A
Unscheduled downtime hours	<10%	<10%	<10%	<10%	N/A
Lujan Neutron Scattering Center	**$2,000**	**$2,000**	**$3,000**	**$3,000**	**$0**
Achieved operating hours	N/A	N/A	N/A	N/A	N/A
Planned operating hours	0	0	0	0	0
Optimal hours	0	0	0	0	0
Percent optimal hours	N/A	N/A	N/A	N/A	N/A
Unscheduled downtime hours	N/A	N/A	N/A	N/A	N/A
Spallation Neutron Source	**$181,425**	**$181,425**	**$198,226**	**$193,209**	**-$5,017**
Number of Users	800	845	850	850	0
Achieved operating hours	N/A	4,441	N/A	N/A	N/A
Planned operating hours	4,700	4,700	4,650	4,700	+50
Optimal hours	4,700	4,700	4,700	4,700	0
Percent optimal hours	100%	94.5%	98.9%	100%	N/A
Unscheduled downtime hours	<10%	<10%	<10%	<10%	N/A

[a] Optimal hours for LCLS are adjusted from 4,700 to 3,000 hours in FY 2017 to allow the facility to conduct transition activities required for LCLS-II.

	FY 2015 Enacted	FY 2015 Current	FY 2016 Enacted	FY 2017 Request	FY 2017 vs FY 2016
TYPE B FACILITIES					
Center for Nanoscale Materials	**$23,427**	**$23,852**	**$24,481**	**$25,205**	**+724**
Number of users	470	529	500	500	0
Center for Functional Nanomaterials	**$19,908**	**$19,908**	**$20,804**	**$21,418**	**+$614**
Number of users	400	493	420	450	+30
Molecular Foundry	**$26,403**	**$26,403**	**$27,591**	**$28,406**	**+$815**
Number of users	470	677	500	500	0
Center for Nanophase Materials Sciences	**$22,901**	**$23,752**	**$23,932**	**$24,638**	**+$706**
Number of users	440	575	450	500	+50
Center for Integrated Nanotechnologies	**$21,010**	**$21,010**	**$21,955**	**$22,605**	**+650**
Number of users	400	513	420	450	+30
Total, All Facilities	**$804,948**	**$810,078**	**$865,314**	**$872,508**	**+$7,194**
Number of Users	13,110	14,587	13,970	13,880	-90
Achieved operating hours	N/A	30,258	N/A	N/A	N/A
Planned operating hours	30,100	30,100	31,450	29,900	-1,550
Optimal hours	30,900	30,900	31,900	29,900	-2,000
Percent of optimal hours	97.9%	96.5%	98.7%	100%	N/A
Unscheduled downtime hours	<10%	<10%	<10%	<10%	N/A

Scientific Employment

	FY 2015 Enacted	FY 2015 Current	FY 2016 Enacted	FY 2017 Estimate	FY 2017 vs FY 2016
Number of permanent Ph.D.'s (FTEs)	4,300	4,300	4,340	4,830	+490
Number of postdoctoral associates (FTEs)	1,110	1,110	1,120	1,320	+200
Number of graduate students (FTEs)	1,670	1,670	1,670	2,030	+360
Other[a]	2,840	2,840	2,900	3,060	+160

[a] 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 2016 CPDS and does not include a new start for FY 2017.

The FY 2017 Request for the Linac Coherent Light Source-II (LCLS-II) is $190,000,000, $10,300,000 less than the FY 2016 Enacted level of $200,300,000. In April 2015, the Office of Science (SC) conducted an external Independent Project Review (IPR) to assess the project's readiness for CD-3B, Approve Long Lead Procurements. The IPR committee found that the project was making good progress overall, but needed to increase the cryoplant refrigeration capacity to address technical risks. In response to this recommendation, the project team proposed increasing the scope of the project by increasing the cryoplant cooling capacity to mitigate the highest technical risk. The Basic Energy Sciences (BES) program accepted the proposal. This change in scope, which includes additional commissioning costs and a larger building to house the additional cryogenic equipment, increased the preliminary total project cost (TPC) point estimate from $965,000,000 to $1,045,000,000. CD-4 is estimated for the third quarter of FY 2022. CD-3B was approved on May 28, 2015, which authorized long lead and advanced procurements for key components of the cryoplant and the superconducting linac which are on the critical path for the project.

Summary
The most recent DOE 413.3B approved Critical Decision (CD) is a revised CD-3B, Approve Long Lead Procurements, that was approved on May 28, 2015. The TPC range of $750,000,000-$1,200,000,000 has not changed.

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

The 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. A liquid helium refrigeration plant is required to cool the linac to superconducting temperatures and a building will be constructed to house the refrigeration plant equipment.

FY 2015 activities included design, long lead and advance procurements (LLP/APs) of critical systems, R&D, prototyping, fabrication, and installation activities. FY 2016 funding will continue activities for design, LLP/APs, R&D, prototyping, site preparation activities (which includes the removal of original linac equipment), fabrication, installation, and initiate construction activities after CD2/CD3 approval is received. FY 2017 funding will be critical for the procurement of materials and equipment needed to maintain the project schedule and expand the construction efforts. Design, LLP/APs, R&D, prototyping, site preparation activities, fabrication, and installation will also continue in FY 2017.

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	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

(fiscal quarter or date)

	CD-0	Conceptual Design Complete	CD-1	CD-2	Final Design Complete	CD-3	D&D Complete	CD-4
FY 2017[a]	4/22/2010	1/21/2014	8/22/2014	2Q FY 2016	4Q FY 2017	2Q FY 2016	N/A	3Q FY 2022

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[b]	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	3Q FY 2015
FY 2017	2Q FY 2016	3/14/2014	5/28/2015

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	47,000	799,400	846,400	48,600	N/A	48,600	895,000
FY 2016	47,000	869,400	916,400	48,600	N/A	48,600	965,000
FY 2017[a,c]	47,000	946,100	993,100	51,900	N/A	51,900	1,045,000

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^{12} x-ray photons in a pulse with duration in the range of 3–500 femtoseconds. These characteristics of the LCLS have opened new realms of research in the chemical, material, and biological sciences. LCLS-II will

[a] This project is pre-CD-2; the estimated cost and schedule are preliminary. Construction will not be executed without appropriate CD approvals.
[b] 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.
[c] 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.

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.

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 free electron laser (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 scope of the LCLS-II project is based on the July 2013 Basic Energy Sciences Advisory Committee (BESAC) report and 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 cryogenic cooling to operate the linac at superconducting temperatures. The increased cryogenic capacity will require increasing the cryogenic equipment building size to approximately 20,000 square foot.

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 $1,045M.

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. In FY 2015, only

about 20% of the experiment proposals received beam time. The addition of a second x-ray source will allow two or more experiments to be run simultaneously. The revised LCLS-II presented here is informed by the 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 is being conducted in accordance with the project management requirements in DOE O 413.3B, Program and Project Management for the Acquisition of Capital Assets.

Key Performance Parameters (KPPs)

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

Preliminary LCLS-II Key Performance Parameters

Performance Measure	Threshold	Objective
Variable gap undulators	2 (soft and hard x-ray)	2 (soft and hard x-ray)
Superconducting linac-based FEL system		
Superconducting linac electron beam energy	3.5 GeV	≥ 4 GeV
Superconducting linac repetition rate	93 kHz	929 kHz
Superconducting linac charge per bunch	0.02 nC	0.1 nC
Photon beam energy range	250–3,800 eV	200–5,000 eV
High repetition rate capable end stations	≥ 1	≥ 2
FEL photon quantity (10^{-3} BW[a])	$5x10^8$ (10x spontaneous @ 2,500 eV)	> 10^{11} @ 3,800 eV
Normal conducting linac-based system		
Normal conducting linac electron beam energy	13.6 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	1,000–15,000 eV	1,000–25,000 eV
Low repetition rate capable end stations	≥ 2	≥ 3
FEL photon quantity (10^{-3} BW[a])	10^{10} (lasing @ 15,000 eV)	> 10^{12} @ 15,000 eV

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

5. Preliminary Financial Schedule

	(dollars in thousands)		
	Appropriations	Obligations	Costs[a]
Total Estimated Cost (TEC)			
Design phase			
MIE funding			
FY 2012	2,000	2,000	2,000
FY 2013[b]	5,000	5,000	5,000
Total, MIE funding	7,000	7,000	7,000
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
Total, Line item construction funding	40,000	40,000	40,000
Total, Design phase	47,000	47,000	47,000
Construction phase			
MIE funding			
FY 2012	42,500[c]	20,000	13,862
FY 2013[b]	17,500	40,000	33,423
FY 2014	0	0	12,256
FY 2015	0	0	455
FY 2016	0	0	4
Total, MIE funding	60,000	60,000	60,000
Line item construction funding			
FY 2014	71,700	71,700	15,213
FY 2015	117,700	117,700	54,531
FY 2016	185,300	185,300	240,300
FY 2017	190,000	190,000	235,000
FY 2018	192,100	192,100	200,000
FY 2019	129,300	129,300	129,300
FY 2020	0	0	11,756
Total, Line item construction funding	886,100	886,100	886,100
Total, Construction phase	946,100	946,100	946,100
TEC			
MIE funding			
FY 2012	44,500[c]	22,000	15,862
FY 2013[b]	22,500	45,000	38,423
FY 2014	0	0	12,256
FY 2015	0	0	455
FY2016	0	0	4
Total, MIE funding	67,000	67,000	67,000

[a] Costs through FY 2015 reflect actual costs; costs for FY 2016 and the outyears are estimates.
[b] FY 2013 funding was requested as a line item, but due to a Continuing Resolution, FY 2013 funds were executed as an MIE.
[c] 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[a]
Line item construction funding			
FY 2014	75,700	75,700	18,713
FY 2015	138,700	138,700	74,531
FY 2016	200,300	200,300	254,800
FY 2017	190,000	190,000	237,000
FY 2018	192,100	192,100	200,000
FY 2019	129,300	129,300	129,300
FY 2020	0	0	11,756
Total, Line item construction funding	926,100	926,100	926,100
Total, TEC[b]	993,100	993,100	993,100
Other Project Cost (OPC)			
OPC except D&D			
MIE funding			
FY 2010	1,126	1,126	938
FY 2011	9,474	9,474	8,033
FY 2012	8,000	8,000	8,893
FY 2013[c]	0	0	116
FY 2014	0	0	439
FY 2015	0	0	10
FY 2016	0	0	171
Total, MIE funding	18,600	18,600	18,600
Line item construction funding			
FY 2014	10,000	10,000	8,142
FY 2015	9,300	9,300	2,650
FY 2016	0	0	4,000
FY 2017	0	0	4,508
FY 2018	7,900	7,900	6,700
FY 2019	6,100	6,100	6,600
FY 2020	0	0	700
Total, Line item construction funding	33,300	33,300	33,300
Total, OPC[b]	51,900	51,900	51,900
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[d]	30,000	24,755
FY 2013[c]	22,500	45,000	38,539
FY 2014	0	0	12,695
FY 2015	0	0	465
FY 2016	0	0	175
Total, MIE funding	85,600	85,600	85,600

[a] Costs through FY 2015 reflect actual costs; costs for FY 2016 and the outyears are estimates.
[b] 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.
[c] FY 2013 funding was requested as a line item, but due to a Continuing Resolution, FY 2013 funds were executed as an MIE.
[d] FY 2012 funding shown includes $22,500,000 of prior year balances from FY 2012 that was reallocated to the LCLS-II project during FY 2013.

	(dollars in thousands)		
	Appropriations	Obligations	Costs[a]
Line item construction funding			
FY 2014	85,700	85,700	26,855
FY 2015	148,000	148,000	77,181
FY 2016	200,300	200,300	258,800
FY 2017	190,000	190,000	241,508
FY 2018	200,000	200,000	206,700
FY 2019	135,400	135,400	135,900
FY 2020	0	0	12,456
Total, Line item construction funding	959,400	959,400	959,400
Total, TPC[b]	1,045,000	1,045,000	1,045,000

6. Details of Project Cost Estimate

	(dollars in thousands)		
	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design			
Design	40,750	37,770	N/A
Contingency	6,250	9,230	N/A
Total, Design	47,000	47,000	N/A
Construction			
Site Preparation	24,700	24,700	N/A
Equipment	672,900	564,800	N/A
Other Construction	58,500	58,500	N/A
Contingency	190,000	221,400	N/A
Total, Construction	946,100	869,400	N/A
Total, TEC[b]	993,100	916,400	N/A
Contingency, TEC	196,250	230,630	N/A
Other Project Cost (OPC)			
OPC except D&D			
Conceptual Planning	1,980	1,980	N/A
Conceptual Design	23,408	23,658	N/A
Research and Development	1,972	1,972	N/A
Start-Up	15,790	11,550	N/A
Contingency	8,750	9,440	N/A
Total, OPC[b]	51,900	48,600	N/A
Contingency, OPC	8,750	9,440	N/A
Total, TPC[b]	1,045,000	965,000	N/A
Total, Contingency	205,000	240,070	N/A

[a] Costs through FY 2015 reflect actual costs; costs for FY 2016 and the outyears are estimates.

[b] 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.

7. Schedule of Appropriations Requests

(dollars in thousands)

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[a] (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
FY 2015	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	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
FY 2017[b]	TEC	142,700	138,700	200,300	190,000	192,100	129,300	0	0	993,100
	OPC	28,600	9,300			7,900	6,100	0	0	51,900
	TPC	171,300	148,000	200,300	190,000	200,000	135,400	0	0	1,045,000

8. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy (fiscal quarter or date)	4Q FY 2021
Expected Useful Life (number of years)	25
Expected Future Start of D&D of this capital asset (fiscal quarter)	4Q FY 2046

(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.

[a] FY 2013 funding was requested as a line item, but due to a Continuing Resolution, FY 2013 funds were executed as an MIE.
[b] 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.

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	~20,000
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"	~20,000
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	~20,000

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^2 and was offset by demolition of a 1,630 ft^2 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.