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. BES research provides the foundations to develop new energy technologies, to mitigate the environmental impacts of energy generation/use, and to support DOE missions in energy, environment, and national security. BES accomplishes its mission through excellence in scientific discovery in the energy sciences, and through stewardship of world-class scientific user facilities that enable cutting-edge research and development.

The research disciplines that BES supports—condensed matter and materials physics, chemistry, geosciences, and aspects of biosciences—touch virtually every important aspect of energy resources, production, conversion, transmission, storage, efficiency, and waste mitigation, providing a knowledge base for achieving a secure and sustainable clean energy future. The 2018 Basic Energy Sciences Advisory Committee (BESAC) report, "A Remarkable Return on Investment in Fundamental Research,"[a] provides key examples of major technological, commercial, and national security impacts directly traceable to BES-supported basic research. This mission-relevance of BES research results from a long-standing established strategic planning process, which encompasses BESAC reports, topical in-depth community workshops and reports, and rigorous program reviews.

BES scientific user facilities consist of a complementary set of intense x-ray sources, neutron sources, and research centers for nanoscale science. Capabilities at BES facilities probe materials and chemical systems 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 science questions. The above-noted BESAC report recounts the central role of these shared resources as a key to U.S. scientific and industrial leadership. In response to the COVID pandemic, BES facilities were at the forefront of the research efforts to understand the virus and to provide therapeutics to combat it. BES has a long history of delivering major construction projects on time and on budget, and of providing reliable availability and support to users for operating facilities. This record of accomplishment begins with rigorous community-based processes for conceptualization, planning, and execution in construction of facilities that continues in performance assessment for operating facilities.

Key to exploiting scientific discoveries for future clean energy systems is the ability to create new materials using sophisticated synthesis and processing techniques, to precisely define the atomic arrangements in matter, and to design chemical processes, which will enable control of physical and chemical transformations and conversions of energy from one form to another. Materials will need to be more functional than today's energy materials, and new chemical processes will require ever-increasing control at the level of electronic structure and dynamics. These advances are not found in nature; rather they must be designed and fabricated to exacting standards using principles revealed by basic science. Today, BES-supported activities are entering a new era in which materials can be built with atom-by-atom precision, chemical processes at the molecular scale can be controlled with increasing accuracy, and computational models can predict the behavior of materials and chemical processes before they have been experimentally realized. Collectively, these new tools and capabilities convey a significant strategic advantage for the Nation to advance the scientific frontiers while laying the foundation for future innovations and economic prosperity.

Highlights of the FY 2022 Request

The BES FY 2022 Request of $2,300.0 million is an increase of $55.0 million, or 2.4 percent, above the FY 2021 Enacted level. The Request focuses resources on the highest priorities in early-stage fundamental research, in operation and maintenance of scientific user facilities, and in facility upgrades.

[a] https://science.osti.gov/~/media/bes/pdf/BESat40/BES_at_40.pdf

Key elements in the FY 2022 Request are summarized below.

Research

The Request continues funding for the Energy Frontier Research Centers (EFRCs), the Batteries and Energy Storage Energy Innovation Hub and the Fuels from Sunlight Hub awards, and the National Quantum Information Science (QIS) Research Centers. BES will build stronger programs with underrepresented institutions and regions, including strengthening awareness in order to address environmental justice issues.

Core research priorities in the FY 2022 Request include:

- Clean Energy: Research to provide understanding and foundations for clean energy crosses the entire portfolio. A few examples:
  - Direct air capture of carbon dioxide: Designing high-selectivity, high-capacity, and high-throughput chemical separations and materials;
  - Hydrogen, Solar: Improved conversion of solar energy to useful energy—and fuels, such as hydrogen by water splitting; and
  - Energy Storage: New materials and chemistries for next-generation electrical and thermal energy storage.
- Critical Materials/Minerals: Critical materials/minerals, including rare earth and platinum-group elements, are vital to the Nation's security and economic prosperity, as well as applications for clean energy. In BES, the Request continues support for research to advance our understanding of fundamental properties of these materials, to identify methodologies to reduce their use and to discover substitutes, and to enhance extraction, chemical processing and separation science for rare earths and platinum-group elements.
- Fundamental Science to Transform Advanced Manufacturing (Advanced Manufacturing): BES invests in fundamental science underpinning advanced manufacturing, partnering across SC, with thrusts in circular, clean, and scalable synthesis and processing; transformational operando characterization; multiscale models and tools; and co-design of materials, processes, and products for functionality and use.
- Revolutionizing Polymer Upcycling: Related to Advanced Manufacturing, BES continues its investment in fundamental research that can provide the foundational knowledge for polymer upcycling, that is, the selective deconstruction of the polymers that constitute plastics, followed by reassembly into high-value chemicals, fuels, or materials in a repeating cycle. Areas of focus include transformative chemistry and biology for polymer upcycling, design of next-generation polymeric materials, and next-generation tools for elucidating chemical and biological mechanisms.
- Microelectronics: Also related to Advanced Manufacturing, BES continues its investment in microelectronics with a focus on materials, chemistry, and fundamental device science. BES will partner with Advanced Scientific Computing Research (ASCR), High Energy Physics (HEP), Nuclear Physics (NP), and Fusion Energy Sciences (FES) to support multi-disciplinary microelectronics research to accelerate the advancement of microelectronic technologies in a co-design innovation ecosystem in which materials, chemistries, devices, systems, architectures, algorithms, and software are developed in a closely integrated fashion.
- Artificial Intelligence and Machine Learning (AI/ML): The Request continues investments in data science and AI/ML to accelerate fundamental research for the discovery of new chemical mechanisms and material systems with exceptional properties and function and to apply these techniques for effective user facility operations and interpretation of massive data sets.
- Exascale Computing Crosscut: The Request continues support for computational materials and chemical sciences to deliver shared software infrastructure to the research communities as part of the Exascale Computing Crosscut.
- Integrated Computational & Data Infrastructure: Partnering with ASCR, BES invests in cost-effective computational, networking, and storage capabilities to keep pace with exponential increases in data rates, volumes, and complexities, including those from scientific user facilities.
- Biopreparedness Research Virtual Environment (BRaVE): In support of the activity, which brings DOE laboratories together to tackle problems of pressing national importance, BES research will focus on developing and maintaining capabilities at user facilities related to biotechnology for responsiveness to biological threats and development of advanced instrumentation to address these research challenges.
- Quantum Information Science (QIS): In support of the National Quantum Initiative, SC QIS Research Centers established in FY 2020 constitute an interdisciplinary partnership among SC programs. This partnership complements a robust core

research portfolio stewarded by the individual SC programs to create the ecosystem across universities, national laboratories, and industry that is needed to advance developments in QIS and related technology.

- Accelerator Science and Technology Initiative: Accelerator R&D is a core capability, which SC stewards for the Nation. Increased support for this initiative will allow the U.S. to continue to provide the world's most comprehensive and advanced accelerator-based facilities for scientific research, and to continue to attract and train the workforce needed to design and operate these facilities.
- Reaching a New Energy Sciences Workforce (RENEW): The Office of Science is fully committed to advancing a diverse, equitable, and inclusive research community key to providing the scientific and technical expertise for U.S. scientific leadership. Toward that goal, BES will participate in the SC-wide RENEW initiative that leverages SC's world-unique national laboratories, user facilities, and other research infrastructures to provide undergraduate and graduate training opportunities for students and academic institutions not currently well represented in the U.S. S&T ecosystem. This includes Minority Serving Institutions and individuals from groups historically underrepresented in STEM, but also includes students from communities with environmental justice impacts and the Established Program to Stimulate Competitive Research (EPSCoR) jurisdictions. The hands-on experiences gained through the RENEW initiative will open new career avenues for the participants, forming a nucleus for a future pool of talented young scientists, engineers, and technicians with the critical skills and expertise needed for the full breadth of SC research activities, including DOE national laboratory staffing.

Facility Operations

In the Scientific User Facilities subprogram, BES maintains a balanced suite of complementary tools. The Advanced Light Source (ALS), Advanced Photon Source (APS), National Synchrotron Light Source-II (NSLS-II), Stanford Synchrotron Radiation Lightsource (SSRL), and Linac Coherent Light Source (LCLS) will continue operations and are supported at approximately 97 percent of optimum. Both BES-supported neutron sources, the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR), will be operational in FY 2022 and funded at approximately 96 percent of optimum. The Request provides funding for the five Nanoscale Science Research Centers (NSRCs) at a level of approximately 96 percent of optimal.

Projects

The Request provides continuing support for the Advanced Photon Source Upgrade (APS-U), Advanced Light Source Upgrade (ALS-U), Linac Coherent Light Source-II (LCLS-II), Linac Coherent Light Source-II High Energy (LCLS-II-HE), Proton Power Upgrade (PPU), Second Target Station (STS), and Cryomodule Repair and Maintenance Facility (CRMF) projects. The FY 2022 Request also continues two Major Item of Equipment projects: NSLS-II Experimental Tools-II (NEXT-II) and NSRC Recapitalization.

Basic Energy Sciences
FY 2022 Research Initiatives

Basic Energy Sciences supports the following FY 2022 Research Initiatives.

(dollars in thousands)

	FY 2020 Enacted	FY 2021 Enacted	FY 2022 Request	FY 2022 Request vs FY 2021 Enacted
Accelerator Science and Technology Initiative	–	5,000	13,000	+8,000
Artificial Intelligence and Machine Learning	10,000	20,000	20,000	–
Biopreparedness Research Virtual Environment (BRaVE)	–	–	9,500	+9,500
Critical Materials/Minerals	–	17,000	25,000	+8,000
Exascale Computing Crosscut	26,000	26,000	26,000	–
Fundamental Science to Transform Advanced Manufacturing	–	–	17,000	+17,000
Integrated Computational & Data Infrastructure	–	–	10,000	+10,000
Microelectronics	5,000	15,000	30,000	+15,000
Quantum Information Science	72,270	92,050	102,000	+9,950
Reaching a New Energy Sciences Workforce (RENEW)	–	–	5,000	+5,000
Revolutionizing Polymers Upcycling	–	8,250	8,250	–
Total, Research Initiatives	**113,270**	**183,300**	**265,750**	**+82,450**

Basic Energy Sciences
Funding

(dollars in thousands)

	FY 2020 Enacted	FY 2021 Enacted	FY 2022 Request	FY 2022 Request vs FY 2021 Enacted
Basic Energy Sciences				
Scattering and Instrumentation Sciences Research	71,235	74,031	85,675	+11,644
Condensed Matter and Materials Physics Research	144,963	170,200	187,769	+17,569
Materials Discovery, Design, and Synthesis Research	65,443	71,189	88,047	+16,858
Established Program To Stimulate Competitive Research EPSCoR	24,088	25,000	25,000	–
Energy Frontier Research Centers - Materials	57,500	57,500	64,678	+7,178
Materials Sciences and Engineering - Energy Innovation Hubs	24,088	24,088	25,000	+912
Computational Materials Sciences	13,000	13,000	13,492	+492
Materials Sciences and Engineering, SBIR/STTR	15,165	–	–	–
Total, Materials Sciences and Engineering	**415,482**	**435,008**	**489,661**	**+54,653**
Fundamental Interactions Research	101,567	107,904	124,415	+16,511
Chemical Transformations Research	97,836	112,292	117,725	+5,433
Photochemistry and Biochemistry Research	75,724	82,589	106,871	+24,282
Energy Frontier Research Centers - Chemical	57,500	57,500	64,678	+7,178
Chemical Sciences, Geosciences, and Biosciences - Energy Innovation Hubs	20,000	20,000	20,758	+758
Chemical Sciences, Geosciences, and Biosciences - General Plant Projects	1,000	1,000	1,000	–
Computational Chemical Sciences	13,000	13,000	13,492	+492
Chemical Sciences, Geosciences, and Biosciences, SBIR/STTR	13,851	–	–	–
Total, Chemical Sciences, Geosciences, and Biosciences	**380,478**	**394,285**	**448,939**	**+54,654**

(dollars in thousands)

	FY 2020 Enacted	FY 2021 Enacted	FY 2022 Request	FY 2022 Request vs FY 2021 Enacted
X-Ray Light Sources	518,791	525,000	538,282	+13,282
High-Flux Neutron Sources	289,701	292,000	293,871	+1,871
Nanoscale Science Research Centers	138,687	139,000	142,387	+3,387
Other Project Costs	23,000	19,000	14,300	-4,700
Major Items of Equipment	10,500	10,500	30,000	+19,500
Scientific User Facilities, Research	39,879	41,207	38,360	-2,847
Scientific User Facilities, SBIR/STTR	36,482	–	–	–
Total, Scientific User Facilities (SUF)	**1,057,040**	**1,026,707**	**1,057,200**	**+30,493**
Subtotal, Basic Energy Sciences	**1,853,000**	**1,856,000**	**1,995,800**	**+139,800**
Construction				
21-SC-10, Cryomodule Repair & Maintenance Facility, (CRMF), SLAC	–	1,000	1,000	–
19-SC-14, Second Target Station (STS), ORNL	20,000	29,000	32,000	+3,000
18-SC-10, Advanced Photon Source Upgrade (APS-U), ANL	170,000	160,000	101,000	-59,000
18-SC-11, Spallation Neutron Source Proton Power Upgrade (PPU), ORNL	60,000	52,000	17,000	-35,000
18-SC-12, Advanced Light Source Upgrade (ALS-U), LBNL	60,000	62,000	75,100	+13,100
18-SC-13, Linac Coherent Light Source-II-High Energy (LCLS-II-HE), SLAC	50,000	52,000	50,000	-2,000
13-SC-10 - Linac Coherent Light Source-II (LCLS-II), SLAC	–	33,000	28,100	-4,900
Subtotal, Construction	**360,000**	**389,000**	**304,200**	**-84,800**
Total, Basic Energy Sciences	**2,213,000**	**2,245,000**	**2,300,000**	**+55,000**

SBIR/STTR funding:

- FY 2020 Enacted: SBIR $57,423,000 and STTR $8,075,000
- FY 2021 Enacted: SBIR $56,592,000 and STTR $7,963,000
- FY 2022 Request: SBIR $59,865,000 and STTR $8,432,000

Basic Energy Sciences
Explanation of Major Changes

	(dollars in thousands) FY 2022 Request vs FY 2021 Enacted
Materials Sciences and Engineering Research will continue to support fundamental scientific opportunities for materials innovations, including those identified in recent BESAC and Basic Research Needs workshop reports. Research priorities include clean energy (e.g., hydrogen, direct air capture, energy storage), critical materials/minerals, exascale (computational materials sciences), data science and AI/ML, integrated computational and data infrastructure, advanced manufacturing, microelectronics, BRaVE, QIS, strategic accelerator technology, and RENEW. The Request also includes funding for continued support of the EFRCs, the Batteries and Energy Storage Energy Innovation Hub, the National QIS Research Centers, and the Established Program to Stimulate Competitive Research (EPSCoR).	**+$54,653**
Chemical Sciences, Geosciences, and Biosciences Research will continue to support fundamental scientific opportunities for innovations in chemistry, geosciences and biosciences, including those identified in recent BESAC, Basic Research Needs, and Roundtable workshop reports. Research priorities include clean energy (e.g., energy efficient, sustainable cycles for carbon and hydrogen, and direct air capture of carbon dioxide), critical materials/minerals, exascale (computational chemical sciences), data science and AI/ML, integrated computational and data infrastructure, advanced manufacturing, polymer upcycling, microelectronics, QIS, and RENEW. The Request also includes funding for continued support of the EFRCs, the Fuels from Sunlight Hub awards, and the National QIS Research Centers.	**+$54,654**
Scientific User Facilities (SUF) The Advanced Light Source (ALS), Advanced Photon Source (APS), National Synchrotron Light Source-II (NSLS-II), Stanford Synchrotron Radiation Lightsource (SSRL), and Linac Coherent Light Source (LCLS) user facilities will operate at approximately 97 percent of optimum. Both BES-supported neutron sources, the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR), will operate at approximately 96 percent of optimum. These facilities will support the BRaVE initiative to maintain capabilities to tackle biological threats. The Request continues to support all five NSRCs at approximately 96 percent of optimum, with funding for continued QIS-related tools development. Research priorities include accelerator science and technology and applications of data science and AI/ML techniques to accelerator optimization, control, prognostics, and data analysis. The Request also continues two major items of equipment: the NEXT-II beamline project for NSLS-II and the NSRC recapitalization project.	**+$30,493**
Construction The Request provides continuing support for the Advanced Photon Source-Upgrade (APS-U), the Advanced Light Source Upgrade (ALS-U), the Linac Coherent Light Source-II (LCLS-II), the Linac Coherent Light Source-II High Energy (LCLS-II-HE), the SNS Proton Power Upgrade (PPU), the SNS Second Target Station (STS), and the Cryomodule Repair and Maintenance Facility at SLAC.	**-$84,800**
Total, Basic Energy Sciences	**+$55,000**

Basic and Applied R&D Coordination

As a program that supports fundamental scientific research relevant to many DOE mission areas, BES strives to build and maintain close connections with other DOE program offices. BES coordinates with 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. BES also coordinates with DOE technology offices in the Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) program, including topical area planning, solicitations, reviews, and award recommendations.

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 polymer upcycling; biofuels derived from biomass; solar energy utilization, including solar fuels; hydrogen production, storage, transport and use; carbon dioxide removal including direct air capture; energy storage; critical minerals/materials; advanced nuclear energy systems; vehicle technologies; biotechnology; and fundamental science to transform advanced manufacturing and industrial processes. These activities facilitate cooperation and coordination between BES and the DOE technology offices and defense programs. Additionally, DOE technology office personnel participate in reviews of BES research, and BES personnel participate in reviews of research funded by the technology offices. DOE leadership has established formal Science and Energy Technology Teams that cross the Department and meet on a regular basis to discuss R&D activities and goals.

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 DOE national laboratory system plays a crucial role in achieving integration of basic and applied research.

Program Accomplishments

Foundational understanding and characterization of novel materials and molecular systems for use in microelectronics and quantum information science.

Future generations of energy-efficient quantum, optical, and electronic devices will be built from advanced materials and molecules that have not previously been exploited technologically. Harnessing the full potential of these systems requires detailed understanding and control of their fundamental properties at the level of atoms and electrons.

- Using neutron diffraction and inelastic scattering, researchers discovered evidence of a long-sought quantum spin liquid (QSL) state that can be controlled with magnetic fields. QSLs are an exotic new phase of matter that may have use as quantum bits (qubits) in quantum information-based applications, and may help scientists understand high-temperature superconductivity and entangled correlated electrons. This discovery, enabled by the unique sensitivity of neutrons to magnetic properties, may provide a foundation to develop materials for applications such as topologically protected qubits, robust against local disorder and perturbations.
- A novel characterization method was used to correlate the optical properties of atomic-defect-based quantum emitters with their atomic and crystallographic structure. The work combined multiple characterization techniques: photoluminescence, cathodoluminescence, and nano-beam electron diffraction. Next-generation quantum and energy technologies will require bright, controllable emitter characteristics and placement. This research provides a foundation for creating such emitters based on atomic “defects-by-design”.
- Using a new technology developed for scanning transmission electron microscopy, researchers produced the most accurate 3D images of 2D materials to date, mapping the materials’ atomic structure to picometer-scale (one-trillionth of a meter) precision. They quantified defects and the effects of doping in the materials, both of which can affect the materials’ electronic properties. This approach should enable scientists to better predict and discover new physical, chemical, and electronic properties of 2D materials at the single-atom level.
- Scientists developed a general, practical approach to test for the presence and degree of entanglement—a key quantum phenomenon exploited in QIS technologies—in continuous measurements of systems such as chemical reactions. An effective procedure to prepare and measure entanglement to uncover how chemical reactions work could enable innovative schemes to mimic or recreate the reactions in new technologies.

Ultrafast chemical and materials sciences.
Advances in science and technology over the past century have been driven by an improved understanding of matter on ever-decreasing length scales, reaching down to atomic dimensions. Understanding and controlling the interplay between atomic-scale structure and the associated ultrafast dynamical processes, which govern the macroscopic functionality observed in matter, are key to discovery and driving innovation in energy applications.

- Researchers used ultrafast x-ray free-electron-laser (XFEL) pulses to observe the initial ultrafast step in the radiolysis of water—the transfer of a proton from an ionized water molecule to form the chemically aggressive hydroxyl radical. Understanding the role of the molecular environment on the mechanism of this process is critical to developing strategies to suppress radiation damage in chemical and materials systems.
- Using a high-speed "electron camera", scientists simultaneously captured the movements of electrons and nuclei in a molecule after it was excited with light. This novel accomplishment used ultrafast electron diffraction, which scatters a short, powerful beam of electrons off matter to reveal tiny molecular motions.
- Information on how light is absorbed and on tracking of energy flows from light to electrons to atoms, including atomic distortions on ultrafast time scales, is needed to understand and control the novel properties of 2D materials. Atomic vibrations in a single molecular sheet were measured by intense pulses in a new time-resolved ultrafast technique using an XFEL. This is now possible at the time and distance limits of the ultrafast dynamics involving particles and arrangements that make up new materials and involve new properties.
- Scientists used ultra-broadband 2D electronic spectroscopy to uncover the ultrafast processes and energy-dissipating mechanisms that prevent damage to molecular systems in plant photosynthesis. This work confirmed a predicted pathway for energy transfer from chlorophyll to carotenoid and suggested a role for the local molecular environment in controlling light harvesting and energy dissipation. These insights could inspire innovative strategies to limit damage from excess energy in clean-energy technologies.

Electrochemical mechanisms in systems for energy generation, conversion, and storage.
Discovery of the electrochemical mechanisms in natural and man-made systems enables scientific design of chemical processes and materials to advance electrochemical systems for clean-energy applications, such as photo-electrochemical cells, batteries, and fuel cells, with the potential for significantly improved performance. Understanding the ingenious mechanisms that nature uses to manage such electrochemical processes provides inspiration for designing man-made systems that mimic these processes.

- Recent innovations in catalyst design for electrochemical reduction of CO_2 resulted in significantly higher activity and selectivity than existing catalysts and avoided the need for high pressures and temperatures. Controlling the catalyst microenvironment by introducing a second metal on palladium-based catalysts led to systematic improvements in the electrochemical conversion of CO_2 to synthesis gas with controllable CO/H_2 ratios. This versatile mixture can lead to a variety of environmentally sustainable chemicals.
- Scientists developed a theoretical model for electron bifurcation, an efficient and reversible electro-chemical reaction so far found only in biology. This process takes the energy of two electrons and splits it unequally, creating one electron with energy high enough to drive difficult reactions and one electron for easier ones. The model predicts that steep free energy gradients help nature avoid "short-circuits" and could guide development of innovative reversible and efficient chemical reactions for clean-energy applications.
- The electrochemical storage mechanism at high voltages for state-of-the-art lithium-ion batteries was elucidated using an array of x-ray structural and electronic characterization tools. Researchers identified two primary charge storage mechanisms for nickel-rich metal oxide electrodes. Below 4.25V, the charge is stored by the transition metal atoms, which lose electrons during charging. Above 4.25V, metal-oxygen bonds develop as electrons are removed from the transition metal. The formation of oxygen-oxygen bonds, which has been postulated as the high-voltage mechanism, was not observed. This fundamental understanding of microscopic mechanisms could help inform future battery design.
- Researchers developed an electrochemical mechanism to protect against unwanted reactions at the electrode-electrolyte interface in lithium-sulfur (Li-S) batteries. Adding small amounts of tellurium to the sulfur cathode or electrolyte significantly improved cycling efficiencies and the number of lifetime charge/discharge cycles (up to 7x improvement). This highlights the potential for a simple and scalable path forward to realize viable, long-lived, high-energy-density Li-S batteries.

New techniques and capabilities at BES facilities.
Recent developments and upgrades at the scientific user facilities provide users with advanced capabilities, especially adopting data science approaches, to conduct cutting-edge science.

- LCLS has successfully delivered coherent x-rays through the newly installed hard x-ray undulator. This new hard x-ray undulator system, developed by the Advanced Photon Source, is the world's first adjustable horizontal gap system for XFELs that can produce vertically polarized x-rays. The energy of the emitted x-rays can be easily changed by tuning the undulator gap to match the needs of an experiment. These unique capabilities provide new scientific research opportunities to a wide range of user communities.
- A data science algorithm was developed that learns from experience and from physical models to reduce the tuning time of a dozen instruments at once for XFEL systems, leading to an optimization of the photon energy that is 65% faster than conventional methods. The reduced machine tuning time frees operators to focus on critical tasks and potentially saves hundreds of hours per year that can be used for different experiments.
- Researchers at a BES neutron source have developed a state-of-the-art capability -- a new 14-tesla magnet with large scattering angle opening and cryogenics to chill samples down to 100 mK. This new sample environment will enable research previously not possible on a broad range of quantum materials and phenomena such as superconductivity, quantum magnetism, and spin liquids.
- A data science technique for nanoscale materials research was developed to visualize and quantify the atomic and molecular structures in three-dimensional samples in real time. The computational efficiency and error sensitivity of the method are suitable for future real-time analysis of data from large characterization facilities.

BES scientific user facilities assist industry to advance technology frontiers, including combating COVID-19.
Industrial researchers used unique capabilities provided by the scientific user facilities to improve advanced manufacturing technologies, and to develop new drugs and vaccines to combat the COVID-19 pandemic.

- Researchers at a BES nanoscale science research center working with their academic and industrial partners have developed and synthesized several designer peptoids (artificial peptides) as potential candidates for COVID-19 vaccines or lung therapeutics. One of these vaccine candidates showed encouraging results in initial testing with animals. Two other peptoid sequences have shown significant activity to prevent viral replication of SARS-CoV-2, which causes COVID-19, in air-interface lung cell cultures.
- X-ray scattering and imaging capabilities provided by BES light sources supported many COVID-19-related research experiments conducted by leading pharmaceutical companies. The most notable results are the structural studies of the proteins of the SARS-CoV-2 virus and their complexes with potential drug candidates. This atomic-resolution 3D structural information is crucial for the development of potential therapeutic drugs and vaccines to fight this pandemic.
- Neutron diffraction and imaging capabilities at a BES neutron source enabled nondestructive characterization of high-resolution structures related to residual stresses in manufactured components, such as complex 3D-printed automobile structures. This data is critical to refine and validate computational modeling as a function of the advanced manufacturing variables, leading to improved efficiency and reliability of the production processes.

Basic Energy Sciences
Materials Sciences and Engineering

Description

Materials are critical to nearly every aspect of energy generation and end-use. Materials limitations are often a significant barrier to improved energy efficiencies, longer lifetimes of infrastructure and devices, or the introduction of new clean energy technologies. The BESAC report on transformative opportunities for discovery science, coupled with the Basic Research Needs workshop reports on energy technologies and roundtable reports, provide further documentation of the importance of materials sciences in forefront research for next-generation scientific and technological advances. The Materials Sciences and Engineering subprogram supports research to provide the fundamental understanding and control 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, theoretical/computational, and instrumentation research that will enable the predictive design and discovery of new materials with novel structures, functions, and properties.

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

- **Scattering and Instrumentation Sciences Research**—Advancing science using new tools and techniques to characterize materials structure and dynamics across multiple length and time scales, including ultrafast science, and to correlate this data with materials performance under real world and extreme conditions.
- **Condensed Matter and Materials Physics Research**—Understanding the foundations of material functionality and behavior including electronic, thermal, optical, mechanical, and rare-earth properties, the impact of extreme environments, and materials whose properties arise from the effects of quantum mechanics.
- **Materials Discovery, Design, and Synthesis Research**—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, including approaches learned from biological systems, that limit the use of rare earth and other critical materials, and that enable more effective polymer chemistries.

The Request continues to focus resources toward the highest-priority fundamental research that supports the DOE mission, including priorities in support of clean energy. The portfolio emphasizes understanding of how to direct and control energy flow in materials systems over multiple time (femtoseconds to seconds) and length (nanoscale to mesoscale and beyond) scales, and translation of this understanding to prediction of material behavior, transformations, and processes in challenging real-world systems, establishing a foundational knowledge base for future advanced, clean energy technologies and advanced manufacturing processes, including extremes in temperature, pressure, stress, photon and radiation flux, electromagnetic fields, and chemical exposures. To maintain leadership in materials discovery, the research supported by this subprogram explores new frontiers of emergent materials behavior; utilization of nanoscale control; and materials systems that are metastable or far from equilibrium. This research includes investigation of the interfaces between physical, chemical, and biological sciences to explore new approaches to novel materials design and advanced manufacturing, including understanding to enable polymer upcycling to higher-value molecular systems. In clean energy-related research, there is a growing emphasis on carbon dioxide removal, including direct capture of carbon dioxide from the air. Other topics in clean energy include a focus on low-carbon hydrogen research and long-duration energy storage. Also, critical materials/minerals research will provide foundational knowledge to enable secure and sustainable supply chains for key clean energy technologies.

Research activities in quantum materials highlight the importance and challenges for materials science in understanding and guiding the development of systems that realize unique properties for quantum information science (QIS). Materials science for microelectronics will provide the needed advances for future computing, sensors, detectors, and communication that are critical for national priorities in energy and for leadership in advanced research over a wide range of fields. An increasingly important aspect of materials research is the use of data science techniques to enhance the utility of both theoretical and experimental data for predictive design and discovery of materials. As an essential element of this research, this subprogram supports the development of advanced characterization tools, instruments, and techniques that can assess a wide range of space and time scales, especially in combination and under dynamic *operando* conditions to analyze non-equilibrium materials, conditions, and excited-state phenomena.

In addition to a diverse portfolio of single-investigator and small-group research projects, this subprogram supports Computational Materials Sciences, Energy Frontier Research Centers (EFRCs), the Batteries and Energy Storage Hub, and SC QIS Centers (in partnership with other SC programs). These research modalities support multi-investigator, multi-disciplinary research focused on forefront scientific challenges in support of the DOE energy mission. This subprogram also includes the DOE Established Program to Stimulate Competitive Research (EPSCoR). The DOE EPSCoR program will strengthen investments in early-stage clean energy research for U.S. states and territories that do not historically have large federally-supported academic research programs, expanding DOE research opportunities to a broad and diverse scientific community. This subprogram also supports the RENEW initiative to provide undergraduate and graduate training opportunities for students and academic institutions not currently well represented in the U.S. S&T ecosystem.

<u>Scattering and Instrumentation Sciences Research</u>
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 nanoscale levels. Research in Scattering and Instrumentation Science supports innovative techniques and instrumentation development for advanced materials science research with scattering, spectroscopy, and imaging using electrons, neutrons, and x-rays, including development of science to understand ultrafast dynamics. These techniques provide precise and complementary information about the relationship among structure, dynamics, and properties, generating scientific knowledge that is foundational to the BES mission. The major advances in materials sciences from DOE's world-leading electron, neutron, and x-ray scattering facilities provide continuing evidence of the importance of this research field. In addition, the BESAC report on transformative opportunities for discovery science identified imaging as one of the pillars for future transformational advances. The use of multimodal platforms to reveal the most critical features of a material has been a finding in several of the Basic Research Needs reports. These tools and techniques are also critical in advancing understanding and discovery of novel quantum materials, including materials for next-generation systems to advance QIS and support the work of SC QIS Centers. This program is focused on open questions in materials science and physics, but these characterization tools are broadly applicable to other fields including chemistry, biology, and geoscience, and can be a key component in preparedness for biological threats.

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 many orders of magnitude. A distinct aspect of this activity is the development of innovative instrumentation and techniques for scattering, spectroscopy, and imaging needed to link the microscopic and macroscopic properties of energy materials, including the use of cryogenic environments to evaluate properties only occurring at these temperatures and to learn about processes and interfaces in materials that are damaged by the probes used to characterize them. The use of multiscale and multimodal techniques to extract heretofore unattainable information on multiple length and time scales is a growing aspect of this research, as is the development and application of cryogenic electron microscopy for challenges in physical sciences. For example, to aid in the design of transformational new materials for clean energy technologies such as batteries, *operando* experiments contribute to understanding the atomic and nanoscale changes that lead to materials failure in non-equilibrium and extreme environments (temperature, pressure, stress, radiation, magnetic fields, and electrochemical potentials). Advances in cryogenic microscopy will support the BRaVE initiative since this instrumentation is heavily used to characterize biological threats. Information from these characterization tools is the foundation for the creation of new materials that have extraordinary tolerance and can function in extreme environments without property degradation.

<u>Condensed Matter and Materials Physics Research</u>
This activity supports fundamental experimental and theoretical research to discover, understand, and control novel phenomena in solid materials, generating scientific knowledge that is foundational to the BES mission. These electronic, magnetic, optical, thermal, and structural materials make up the infrastructure for clean energy technologies, as well as accelerator and detector technologies for SC facilities. Also supported is research to understand the role of rare earth and other critical materials in determining functionality, so that they can be reduced or eliminated from key energy technology supply chains.

Experimental research in this program emphasizes discovery and characterization of materials' properties that have the potential to be exploited for new technological functionalities. Complementary theoretical research aims to explain such properties across a broad range of length and time scales. Theoretical research also includes development and integration of predictive theory and modeling for discovery of materials with targeted properties. Advanced computational and data science techniques (including artificial intelligence and machine learning) are increasingly enabling knowledge to be extracted from large materials databases of theoretical calculations and experimental measurements. This program also supports the development of such databases as well as the computational tools that can take advantage of them.

This program continues to emphasize understanding and control of quantum materials whose properties result from interactions of the constituent electrons with each other, the atomic lattice, or light. Investigations include bulk materials as well as 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 advances the fundamental understanding of electronic, magnetic, and optical properties relevant to energy-efficient microelectronics and quantum information science (QIS). The focus on QIS research couples experimental and theoretical expertise in quantum materials with prototypes of quantum structures that can be used to study the science of device functionality and performance.

Activities also emphasize research to understand how materials respond to temperature, light, radiation, corrosive chemicals, and other environmental conditions. This includes electrical and optical properties of materials related to solar energy as well as the effects of defects on electronic properties, strength, deformation, and failure over a wide range of length and time scales. A recent focus is on extending knowledge of radiation effects to enable predictive capabilities for the extreme environments expected in future nuclear reactors and accelerators for SC facilities.

In FY 2022, BES will continue to partner with other SC programs to support the QIS Centers initiated in FY 2020. These centers focus on a set of QIS applications and cross-cutting topics that span the development space that will impact SC programs, including sensors, communication, quantum emulators/simulators, and enabling technologies that will pave the path to exploit quantum computing in the longer term. Research supported by this program will include theory of materials for quantum applications in computing, communication, and sensing; device science for next-generation QIS systems, including interface science and modeling of materials performance; and synthesis, fabrication, and characterization of quantum materials, including integration into novel device architectures to explore QIS functionality.

In partnership with ASCR, HEP, FES, and NP, BES will continue activities begun in FY 2021 to support multi-disciplinary basic research to accelerate the advancement of microelectronic technologies in a co-design innovation ecosystem, as called for by the Basic Research Needs for Microelectronics report.[a] Among the challenges is discovery science that can lead to low-power microelectronics for edge computing as well as for exascale computers and beyond. Such computing capabilities will be necessary to analyze the vast volumes of data that will be generated by future SC facilities. Similarly, transforming power electronics and the electricity grid into a modern, agile, resilient, and energy-efficient system requires improvements in advanced microelectronics materials, and their integration within a co-design framework.

Materials Discovery, Design, and Synthesis Research

The discovery and development of new materials has long been recognized as the engine that drives science frontiers, technology innovations, and advanced manufacturing. 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, generating scientific knowledge that is foundational to the BES mission.

The BESAC 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. In FY 2022 this program

[a] https://science.osti.gov/-/media/bes/pdf/reports/2019/BRN_Microelectronics_rpt.pdf

will continue to expand the application of materials discovery and synthesis research to understand the unique properties of rare earth and other critical materials/minerals, with the goal of reducing their use. New research directions will be inspired by BES reports related to advanced manufacturing, including polymer upcycling. Understanding of synthesis science will enable design of new systems that are easier to efficiently convert into similar products with comparable or enhanced complexity, functionality, and value. Emphasis will include advancing the basic science of advanced manufacturing through innovative approaches for scalable assembly and integration of predictive modeling with characterization tools tuned to advanced manufacturing scale, complexity, and speed.

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 biology-inspired approaches to design and synthesize novel materials with some of the unique properties found in nature. Major research directions include the controlled synthesis and assembly of nanoscale materials into functional materials with desired properties; mimicking the low-energy synthesis approaches of biology to produce materials; 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 and self-regulating 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 research to understand 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, including the extraordinary challenges for synthesis of quantum materials.

Established Program to Stimulate Competitive Research (EPSCoR)
The DOE EPSCoR program funds early-stage research that supports DOE's energy mission in states and territories with historically lower levels of Federal academic research funding. Eligibility determination for the DOE EPSCoR program follows the National Science Foundation eligibility analysis.

The DOE EPSCoR program emphasizes research that will improve the capability of designated states and territories to conduct sustainable and nationally competitive energy-related research; jumpstart research capabilities in designated states and territories through training scientists and engineers in energy-related areas; and build beneficial relationships between scientists and engineers in the designated jurisdictions and world-class national laboratories managed by the DOE. This research leverages DOE national user facilities and takes advantage of opportunities for intellectual collaboration across the DOE system. Through broadened participation, DOE EPSCoR seeks to augment the network of energy-related research performers across the Nation.

Annual EPSCoR funding opportunities alternate between a focus on research performed in collaboration with the DOE national laboratories and a focus on implementation awards that facilitate larger team awards for the development of research infrastructure in the EPSCoR jurisdictions. The FY 2022 program will focus on EPSCoR State-National Laboratory Partnership awards promoting single PI and small group interactions with the unique capabilities of the DOE national laboratory system and will focus on clean energy research, expanding this important research community. The program supports early career scientists from EPSCoR jurisdictions on an annual basis and provides complementary support for research grants to eligible institutions.

Energy Frontier Research Centers
The EFRC program 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 what is possible in standard single-investigator or small-group awards. These multi-investigator, multi-disciplinary centers foster, encourage, and enable transformative scientific advances. They allow experts from a variety of disciplines to collaborate on shared challenges, combining their strengths to uncover new and innovative solutions to the most difficult problems in materials sciences. The EFRCs also support numerous graduate students and postdoctoral researchers, educating and training a scientific workforce for the 21st century economy. The EFRCs supported in this subprogram focus on the following topics: the design, discovery, synthesis, characterization, and understanding of novel, solid-state materials that convert energy into electricity; the understanding of materials and processes that are foundational for electrical energy storage and gas separation; quantum materials and quantum information science; microelectronics; and materials for future nuclear energy and waste storage.

After eleven years of research activity, the program has produced an impressive breadth of scientific accomplishments, including over 12,700 peer-reviewed journal publications.

BES uses a variety of methods 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. Each EFRC undergoes a review of its management structure and approach in the first year of the award and a midterm assessment of scientific progress compared to its scientific goals. To facilitate communication of results to other EFRCs and DOE, BES holds scientific meetings of the EFRC researchers biennially.

In FY 2022 BES plans to issue a Funding Opportunity Announcement to re-compete the four-year EFRC awards that were made in FY 2018. Emphasis will be placed on clean energy topics and other program priorities.

Energy Innovation Hubs

The Joint Center for Energy Storage Research (JCESR), the Batteries and Energy Storage Hub, focuses on early-stage research to tackle forefront, basic scientific challenges for next-generation electrochemical energy storage. JCESR is a multi-institutional research team led by Argonne National Laboratory (ANL) in collaboration with four other national laboratories, eleven universities, the Army Research Laboratory, and industry. In the initial five-year award (2013-2018), JCESR created a library of fundamental scientific knowledge including: demonstration of a new class of membranes for anode protection and flow batteries; elucidation of the characteristics required for multi-valent intercalation electrodes; understanding the chemical and physical processes that must be controlled in lithium-sulfur batteries to greatly improve cycle life; and computational screening of over 16,000 potential electrolyte compounds using the Electrolyte Genome protocols.

For the current award (2018-2023, pending annual progress reviews and appropriations), JCESR identified critical scientific gaps to serve as a foundation for the research. The research directions are consistent with the priorities established in the 2017 BES workshop report *Basic Research Needs for Next Generation Electrical Energy Storage*[a] including discovery science for exploration of new battery chemistries and materials with novel functionality. JCESR is focusing on advances that will elucidate cross-cutting scientific principles for electrochemical stability; ionic and electronic transport at interfaces/interphases, in bulk materials or membranes; solvation structures and dynamics in electrolytes; nucleation and growth of materials, new phases, or defects; coupling of electrochemical and mechanical processes; and kinetic factors that govern reversible and irreversible reactions. Close coupling of theory, simulation, and experimentation is proving critical to accelerate scientific progress; to unravel the complex, coupled phenomena of electrochemical energy storage; to bridge gaps in knowledge across length and temporal scales; and to enhance the predictive capability of electrochemical models. In the current research, prototypes are being used to demonstrate the impact of materials advances for specific battery architectures and designs.

Based on established best practices for managing large awards, BES will continue to require quarterly reports, frequent teleconferences, and annual progress reports and peer reviews to communicate progress, provide input on the technical directions, and ensure high-quality, impactful research. In FY 2022, JCESR will receive the tenth and final year of funding.

Computational Materials Sciences

Major strides in materials synthesis, processing, and characterization, combined with concurrent advances in computational science—enabled by enormous improvements in high-performance computing capabilities—have opened an unprecedented opportunity to design new materials with specific functions and physical properties. The goal 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 or functionalities, and in turn, create new advanced, innovative technologies. Given the importance of materials to virtually all technologies, including clean energy, computational materials sciences are critical for American competitiveness in advanced manufacturing and global leadership in innovation.

This paradigm shift will accelerate the design of revolutionary materials to enable the Nation's energy and quantum information security, tackle the climate challenge, and enhance economic competitiveness. Success will require extensive

[a] https://science.osti.gov/-/media/bes/pdf/reports/2017/BRN_NGEES_rpt.pdf

R&D with the goal of creating experimentally validated, robust community codes that will enable functional materials innovation.

Awards in this program focus on the creation of computational codes and associated experimental/computational databases for the design of functional materials or quantum materials with new functionalities. This research is performed by small groups and fully integrated teams. Large teams combine the skills of experts in materials theory, modeling, computation, synthesis, characterization, and fabrication. The research includes development of new ab initio theory, contributing the generated data to databases, as well as advanced characterization and controlled synthesis to validate the computational predictions. It uses the unique world-leading tools and instruments at DOE's user facilities. The computational codes will use DOE's leadership computational facilities and be positioned to take advantage of today's petascale and tomorrow's exascale high-performance computers. This will result in open source, robust, validated, user-friendly software that captures the essential physics of relevant materials systems. The goal is the use of these codes and generated data by the broader research community and by industry to accelerate the design of new functional materials.

BES manages the computational materials science research activities using the approaches developed for similar small and large team modalities. Management reviews by a peer review panel are held in the first year of the award for large teams. Mid-term peer reviews are held to assess scientific progress, with regular teleconferences, annual progress reports, and active oversight by BES throughout the performance period.

Activities and Explanation of Changes

(dollars in thousands)

FY 2021 Enacted		FY 2022 Request	Explanation of Changes FY 2022 Request vs FY 2021 Enacted
Materials Sciences and Engineering	**$435,008**	**$489,661**	**+$54,653**
Scattering and Instrumentation Sciences Research	$74,031	$85,675	+$11,644
Funding continues to push the frontiers of instrumentation and techniques needed to understand materials properties and enable materials discovery, including quantum phenomena, materials behavior in extreme energy-related environments, and multidimensional phenomena (requiring simultaneous assessment crossing space, time, and chemical evolution). Investments emphasize hypothesis driven research with x-ray free electron lasers, imaging with coherent x-rays, advanced neutron scattering probes of interfaces and soft materials, cryogenic electron microscopy probes, and multimodal techniques that combine probes. Research focuses on innovation that will enable assessment of new regimes not amenable to current characterization approaches.		The Request will continue to focus on the development and use of advanced characterization tools to address the most challenging fundamental questions in materials science, including quantum behavior and properties. The use of multiscale and multimodal techniques to extract information on multiple length and time scales is a growing emphasis, as is the development and application of cryogenic microscopy techniques to answer open questions in physical sciences. Advanced instrumentation research can be applied to diverse national priorities, including QIS, clean energy science, and preparedness for biological threats.	Funding will emphasize the advancement of novel measurement techniques and application of the tools to a broad range of science challenges, from quantum phenomena in energy materials to soft materials. Expanded investments will include a focus on clean energy research in underrepresented communities and institutions.

(dollars in thousands)

FY 2021 Enacted	FY 2022 Request	Explanation of Changes FY 2022 Request vs FY 2021 Enacted
Condensed Matter and Materials Physics Research $170,200	$187,769	+$17,569
Funding continues to support research to understand, design, and discover new quantum materials, and to advance the theory needed to understand quantum phenomena. Included is a specific focus on research to support QIS and related systems. This activity provides continued support for the QIS Centers established in FY 2020. Investments continue to establish the science base for next-generation optical and electronic materials, including a new emphasis on materials for next-generation microelectronics and for accelerator magnets, optics, and detectors. Support increases for investigations of the unique properties associated with rare earth and critical materials to identify opportunities for substitutions and reduced use of these elements in energy relevant technologies. Theory and modeling research includes AI/ML for data-driven science to enhance materials discovery.	The Request will continue to emphasize the understanding and control of the fundamental properties of materials that are central to their functionality in a wide range of clean energy-relevant technologies, including critical materials/minerals. Exploration of quantum materials remains a high priority, and particularly the role that these materials play in microelectronics, accelerators, and the broad emerging field of QIS. The program will continue to partner with other SC program offices to support the QIS Centers that were initiated in FY 2020. Additional focus areas include the response of materials to environmental conditions, including temperature, light, corrosive chemicals, and radiation. Integration of experimental techniques with theoretical and computational research is a key to success, with an emphasis on new data science techniques.	Funding will enhance clean energy research, critical materials/minerals as well as materials in high-radiation environments including future accelerators. Efforts will also support the development and integration of computational and data science tools to enable scientific discovery. Expanded investments will include a focus on clean energy research in underrepresented communities and institutions.

(dollars in thousands)

FY 2021 Enacted	FY 2022 Request	Explanation of Changes FY 2022 Request vs FY 2021 Enacted
Materials Discovery, Design, and Synthesis Research $71,189	$88,047	+$16,858
Funding continues for research on innovative synthesis and discovery of materials through scientific understanding of the basic chemical and physical phenomena, and science-based utilization of biological concepts. Support is maintained for investigation of fundamental dynamics and kinetics of synthesis and self-assembly over multiple length and timescales, including the role of defects and interfaces. Research emphasizes new approaches to replace or minimize the use of critical and rare earth materials in energy-relevant technologies.	The Request will continue support for the design, discovery, and synthesis of novel forms of matter with desired properties and functionalities with an emphasis on advancing the fundamental science relevant to future advanced manufacturing, including innovative approaches to scalable assembly and integration of characterization and predictive modeling. Research will continue to explore science-based solutions to materials criticality. Research on bio-mimetic and biology-inspired materials is relevant to energy technologies as well as other national priorities such as preparedness for and response to biological threats.	The scientific focus will continue to evolve in response to research directions identified in recent strategic planning activities, such as the 2020 Basic Research Needs Workshop for Transformative Manufacturing. Expanded investments will include a focus on clean energy research in underrepresented communities and institutions.
Established Program to Stimulate Competitive Research (EPSCoR) $25,000	$25,000	$ —
Funding continues to support early stage science, including research that underpins DOE energy technology programs. Following the previous year's focus on state-lab partnership awards, FY 2021 emphasizes implementation awards, larger multiple principal investigator grants that develop research capabilities in EPSCoR jurisdictions. The FY 2021 funding opportunity solicits both renewals of FY 2019 awards and new proposals. Investment continues in early career research faculty from EPSCoR designated jurisdictions and in co-investment with other programs for awards to eligible institutions.	The Request will continue to support early-stage science, including research that underpins DOE energy technology programs. Following the previous year's focus on implementation awards, FY 2022 will emphasize state-lab partnership awards, single principal investigator and small group grants that promote interactions with the unique capabilities and expertise at the DOE National Labs with a technical focus on clean energy research. The FY 2022 funding opportunity will consider new proposals. Investment will continue in early career research faculty from EPSCoR-designated jurisdictions and in co-investment with other programs for awards to eligible institutions.	Funding will focus on State-National Laboratory Partnership awards focused on clean energy research and promoting single PI and small group interactions with the unique capabilities of the DOE national laboratory system.

(dollars in thousands)

FY 2021 Enacted	FY 2022 Request	Explanation of Changes FY 2022 Request vs FY 2021 Enacted
Energy Frontier Research Centers $57,500	$64,678	+$7,178
Funding provides the fourth year of support for four-year EFRC awards that were made in FY 2018 and the second year of support for four-year EFRC awards that were made in FY 2020.	The Request will provide the third year of support for four-year EFRC awards that were made in FY 2020 in the following topical areas: environmental management, microelectronics, and QIS. In addition, BES plans to issue a solicitation in FY 2022 to re-compete the EFRC awards made in FY 2018, with emphasis on clean energy and other high-priority topics.	Technical emphasis for the EFRC program will include research directions identified in recent strategic planning activities and aligned with program priorities. Expanded investments will include a focus on clean energy research in underrepresented communities and institutions.
Energy Innovation Hubs $24,088	$25,000	+$912
Funding continues the prior year's focus, based on the renewal of the JCESR Hub in FY 2018. Early stage research for next generation electrical energy storage for the grid and vehicles continues to emphasize understanding the fundamentals of electrochemistry (transport, solvation, evolution of chemistries and materials during charge/ discharge) and discovery of the coupled factors that govern performance. The research closely integrates theory, simulation, and experimentation to elucidate the impact of coupled phenomena and enable predictive design of new materials for batteries.	The Request will provide the tenth and final year of funding for JCESR. JCESR is focusing on advancing understanding of scientific principles for electrochemical stability; transport in the bulk, at interfaces, and across membranes; coupling electrochemical and mechanical processes; and dynamics that control reversible and irreversible reactions. Tight coupling of theory, simulation, and characterization will accelerate understanding of the complex, coupled phenomena.	Funding will support the final year of funding for JCESR.

(dollars in thousands)

FY 2021 Enacted		FY 2022 Request	Explanation of Changes FY 2022 Request vs FY 2021 Enacted
Computational Materials Sciences	$13,000	$13,492	+$492
Funding continues to support research on current CMS awards that focus on development of research-oriented, open-source, experimentally validated software and the associated databases required to predictively design materials with specific functionality. Software utilizes leadership class computers, and will be made available to the broad research community. The codes incorporate frameworks suited for future exascale computer systems.		The Request will continue research that focuses on development of computational codes and associated experimental and computational databases for the predictive design of functional materials. The research includes development of new ab initio theory, populating databases, and advanced characterization and controlled synthesis to validate the computational predictions. The goal is open source, validated software that uses today's DOE's leadership computational facilities and is poised to take advantage of tomorrow's exascale high-performance computers.	Funding will continue to support research in ongoing CMS Awards.

Note: Funding for the subprogram above, includes 3.65% of research and development (R&D) funding for the Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) Programs.

Basic Energy Sciences
Chemical Sciences, Geosciences, and Biosciences

Description

Understanding and ultimately controlling transformations of energy among forms, and rearrangements of matter across multiple scales starting at the atomic level, are essential to development of innovative clean-energy technologies. The Chemical Sciences, Geosciences, and Biosciences subprogram supports research to discover fundamental knowledge of chemical reactivity and energy conversion that is the foundation for energy-relevant chemical processes, such as catalysis, synthesis, separations, and light-induced chemical transformations. The research addresses the challenge of understanding how physical and chemical phenomena at the scales of electrons, atoms, and molecules control complex and collective behavior of macro-scale energy conversion systems. At the most fundamental level, understanding of quantum mechanical behavior is rapidly evolving into the ability to control and direct such behavior to achieve desired outcomes. This subprogram seeks to extend the new era of control science to include the capability to tailor chemical transformations with atomic and molecular precision. Here, the challenge is to achieve predictive understanding of 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 Research**—Discover the foundational factors controlling chemical reactivity and dynamics in the gas phase, in condensed phases, and at interfaces, based upon a quantum description of the interactions among photons, electrons, atoms, and molecules.
- **Chemical Transformations Research**—Understand and control the mechanisms of chemical catalysis, synthesis, separation, stabilization, and transport in complex chemical systems, from atomic to geologic scales.
- **Photochemistry and Biochemistry Research**—Elucidate the molecular mechanisms of the capture of light energy and its conversion into electrical and chemical energy through biological and chemical pathways.

The Request continues the highest-priority fundamental research, including support of clean energy such as chemistry for low-carbon, efficient, sustainable, and circular approaches to advanced manufacturing. Related research emphasizes chemical upcycling of polymers and the chemistry of rare earth and platinum-group elements important in manufacturing supply chains (critical materials/minerals). Fundamental biochemistry will develop models and datasets for discovery of principles to enable biomimetic and biohybrid clean energy systems. Research focused on molecular science will enable new microelectronics and lead to understanding of the phenomena relevant to QIS and quantum computing. Bringing simulation and experiments together, integration of data science and computational chemistry will provide the needed tools and infrastructure for shared data repositories.

The following five synergistic, foundational research themes are at the intersections of multiple research focus areas in this portfolio. Ultrafast Chemistry probes electron and atom dynamics to understand energy and chemical conversions. Chemistry at Complex Interfaces advances understanding of how the dynamics of interfaces as well as their structural and functional disorder influence chemical phenomena. Charge Transport and Reactivity explores how charge dynamics contribute to energy flow and chemical conversions. Reaction Pathways in Diverse Environments discovers the influence of nonequilibrium, heterogeneous, nanoscale, and extreme environments on complex reaction mechanisms. Chemistry in Aqueous Environments addresses water's unique properties, and the role aqueous systems play in energy and chemical conversions.

The subprogram supports a diverse portfolio of research efforts including single investigators, small groups, and larger multi-investigator, cross-disciplinary teams—through EFRCs, the Fuels from Sunlight Energy Innovation Hub program, Computational Chemical Sciences, Data Science, and QIS—to advance foundational science for development of clean-energy technologies. The subprogram also supports, in partnership with other SC programs, SC QIS Research Centers that were established in FY 2020. This subprogram also supports the RENEW initiative to provide undergraduate and graduate training opportunities for students and academic institutions not currently well represented in the U.S. S&T ecosystem.

Fundamental Interactions Research
This activity emphasizes structural and dynamical studies of atoms, molecules, and nanostructures, and the description of their interactions in full quantum detail. The goal is to achieve a complete understanding of reactive chemistry in the gas phase, in condensed phases, and at interfaces. This activity provides leadership for ultrafast chemistry, supporting research that advances ultrafast tools and approaches, as well as their application to probe and control chemical processes. Research supports theory and computation for accurate and efficient descriptions of molecular reactions and chemical dynamics.

The principal research thrusts in this activity are atomic, molecular, and optical sciences (AMOS), gas phase chemical physics (GPCP), condensed phase and interfacial molecular science (CPIMS), and computational and theoretical chemistry (CTC). AMOS research emphasizes the fundamental interactions of atoms and molecules with ultrafast electrons and photons, to characterize and control their behavior. Novel attosecond sources, x-ray free electron laser sources such as the LCLS, and ultrafast electron diffraction are used to image the dynamics of electrons and charge transport. CPIMS research emphasizes foundational research at the boundary of chemistry and physics, pursuing a molecular-level understanding of chemical, physical, and electron- and photon-driven processes in liquids and at interfaces. Experimental, theoretical, and computational investigations in the condensed phase and at interfaces aim to elucidate the molecular-scale chemical and physical properties and interactions that govern condensed phase structure and dynamics. The GPCP program supports research on fundamental gas-phase chemical processes important in energy applications. Research in this program explores chemical reactivity, kinetics, and dynamics in the gas phase at the level of electrons, atoms, molecules, and nanoparticles. The CTC program supports development, improvement and integration of new and existing theoretical and massively parallel computational or data-driven strategies for the accurate and efficient prediction or simulation of processes and mechanisms. Research in this area is crucial to utilize planned exascale computing facilities and to optimize use of existing petascale computers, leveraging U.S. leadership in the development of open-source computational chemistry codes and databases. In the context of SC QIS Centers, this research also lays the groundwork for applications of future quantum computers to computational quantum chemistry.

In FY 2022, BES, in partnership with other SC programs, will continue support for the multi-disciplinary multi-institutional QIS centers, initiated in FY 2020. The SC QIS centers will focus on a set of QIS applications or cross-cutting topics including innovative research on sensors, quantum emulators/simulators, and enabling technologies that will pave the path to exploit quantum computing in the longer term. Research initiated in FY 2021 in microelectronics will continue with a focus on unraveling complex mechanisms of chemical reactions at interfaces to inform the design and synthesis of new materials.[a] The Fundamental Interactions activity will continue to advance data science and computational approaches for chemical sciences with a focus on integration of databases and computational chemistry tools for the generation of scientific knowledge that is foundational to the BES mission.

Chemical Transformations Research
This activity seeks fundamental understanding of chemical reactivity, matter and charge transport, and chemical separation and stabilization processes that are foundational in core research areas—catalysis science, separation science, heavy element chemistry, and geosciences—which are critical for developing future clean-energy and advanced manufacturing technologies. The research entails use of ultrafast spectroscopy to follow transient species during reactions; advances understanding of charge transport and reactivity, which determine the kinetics of electrocatalytic, separations, and geochemical processes; explores the influence of complex interfaces on chemical transformations; and develops understanding of chemistry in aqueous environments that influence many sustainable chemical processes. Understanding reaction pathways in diverse catalytic, separation and geological environments is a major focus in this activity.

Catalysis science research is focused on understanding reaction mechanisms, precise synthesis, *operando* characterization, manipulation of catalytic active sites and their environments, and control of reaction conditions for efficiency and selectivity. A primary goal is the molecular-level control of chemical transformations relevant to the sustainable conversion of energy resources, with emphasis on thermal and electrochemical conversions. Separation science research seeks to understand and ultimately predict and control the atomic and molecular interactions and energy exchanges determining the efficiency and viability of chemical separations, with emphasis on critical elements and atmospheric CO_2. The major

[a] https://science.osti.gov/-/media/bes/pdf/reports/2019/BRN_Microelectronics_rpt.pdf

focus is to advance discovery of principles and predictive design of future chemical separation approaches with improved efficiencies. Heavy element chemistry provides foundational knowledge on the influence of complex environments, such as multiple phases and extreme conditions of temperature and radiation, on the dynamic behavior of actinide compounds. A primary goal is to advance understanding of the unique chemistry of f-electron systems that is required to design new ligands for actinide separations processes, to predict the chemical evolution of actinides in nuclear wastes and next-generation reactors, and to improve models of actinide environmental transport. Geosciences research provides the fundamental science underlying the subsurface chemistry and physics of natural substances under extreme conditions of pressure or confined environments. Areas of emphasis include the molecular-level understanding of phase equilibria, reaction mechanisms and rates associated with aqueous geochemical processes, and a mechanistic understanding of the origins of subsurface physical properties and the response of earth materials subject to chemo-mechanical stress corrosion and strain localization.

In FY 2022, this activity will continue to support efforts central to transformative approaches to advanced manufacturing,[a] including predictive design of catalytic and separations processes for circular use of natural and synthetic resources with atom and energy efficiency, as exemplified by polymer upcycling—the selective chemical deconstruction of polymers that make up plastics followed by reassembly into high-value products.[b] This activity will increase focus on discovery and design of sustainable cycles for carbon and hydrogen, by means of enhanced carbon separation from dilute as well as concentrated sources and clean-energy cycles of hydrogen generation and use. This activity will also continue to address challenges in critical materials with focus on novel approaches for selective separation, and substitution and use of rare earth and platinum-group elements. Research will continue to investigate the unique quantum phenomena enabled by f-electron elements, which could lead to novel approaches for QIS. Research will develop fundamental knowledge of subsurface processes across spatial and temporal scales—such as mineralization, crack propagation, and rock fracture – that are critical for innovative methods of resource extraction, including critical minerals. The use of data science and AI/ML approaches will continue to be emphasized in research across the portfolio to accelerate the generation of scientific knowledge that is foundational to the BES mission.

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. An important component of this activity is its leadership role in the support of basic research in both solar photochemistry and natural photosynthesis. Innovative research on absorption, transfer, and conversion of energy across spatial and temporal scales and on redox interconversion of small molecules (e.g., carbon dioxide/methane, nitrogen/ammonia, and protons/hydrogen) advances basic understanding of dynamic mechanisms of charge transport and reactivity. Studies of ultrafast chemistry and photo-driven quantum coherence probe the short time-scales critical in natural photosynthesis and artificial molecular systems and can provide insights into the role of quantum phenomena in chemical and biochemical reactions. Crosscutting research on the dynamics and function of enzymes, natural and artificial membranes, and nano- to meso-scale structures provides mechanistic understanding of how complex interfaces and aqueous environments influence reaction pathways and can inspire new strategies for clean energy conversions.

This activity integrates multidisciplinary research at the interface of chemistry, physics, and biology. Research of biological systems provides insights for understanding and enhancing man-made chemical systems. In a reciprocal manner, studies of chemical (non-biological) systems provide insights on the dynamics and reactivity underlying biochemical processes. Research in natural photosynthesis advances knowledge of biological mechanisms of solar energy capture and conversion and can inspire development of bio-hybrid, biomimetic, and artificial photosynthetic systems for clean-energy production. Studies of complex multielectron redox reactions, electron bifurcation, and quantum phenomena in biological systems can suggest innovative approaches to energy conversion and storage strategies for clean-energy applications. Complementary research on the elementary steps of light absorption, charge separation, and charge transport of solar energy conversion in man-made systems provides foundational knowledge for the use of solar energy for fuel production and electricity generation. Research also addresses fundamental effects resulting from ionizing radiation to understand chemical reactions in extreme environments and to provide insights for remediation, fuel-cycle separation, and design of nuclear reactors.

[a] https://science.osti.gov/-/media/bes/pdf/reports/2020/Transformative_Mfg_Brochure.pdf

[b] https://science.osti.gov/-/media/bes/pdf/reports/2020/Chemical_Upcycling_Polymers.pdf

In FY 2022, research will continue to establish a molecular-level understanding of biochemical processes. Efforts will build on BES biochemistry and biophysics research to discover and design chemical processes and complex structures that can enable clean energy innovations for advanced manufacturing and microelectronics, such as bio-inspired, biohybrid, and biomimetic systems with desired functions and properties. Studies of photo-driven quantum coherence in natural photosynthesis and artificial molecular systems will continue with the goal of inspiring new approaches in QIS. Research will also address challenges such as reducing the use of critical and rare earth elements in light absorbers and catalysts for clean energy. Efforts across this research portfolio will continue to generate scientific knowledge that is foundational to the BES mission.

Energy Frontier Research Centers

The EFRC program 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 what is possible in standard single-investigator or small-group awards. These multi-investigator, multi-disciplinary centers foster, encourage, and accelerate basic research to enable transformative scientific advances. They allow experts from a variety of disciplines to collaborate on shared challenges, combining their strengths to uncover new and innovative solutions to the most difficult problems in chemical sciences, geosciences, and biosciences. The EFRCs also support numerous graduate students and postdoctoral researchers, educating and training a scientific workforce for the 21st-century economy. The EFRCs supported in this subprogram focus on the following topics: the design, discovery, characterization, and control of the chemical, biochemical, and geological processes for improved electrochemical conversion and storage of energy; the understanding of catalytic chemistry and biochemistry that are foundational for fuels, chemicals, separations, and polymer upcycling; interdependent energy-water issues; quantum information science; future nuclear energy and the chemistry of waste processing; and advanced interrogation and characterization of the earth’s subsurface. After eleven years of research activity, the program has produced an impressive breadth of scientific accomplishments, including over 12,700 peer-reviewed journal publications.

BES uses a variety of methods 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. Each EFRC undergoes a review of its management structure and approach in the first year of the award and a mid-term assessment by outside experts of scientific progress compared to its scientific goals. To facilitate communication of results to other EFRCs and DOE, BES holds meetings of the EFRC researchers biennially.

In FY 2022 BES plans to issue a Funding Opportunity Announcement to re-compete the four-year EFRC awards that were made in FY 2018. Emphasis will be placed on clean energy topics and other program priorities.

Energy Innovation Hubs

The two multi-investigator, cross-disciplinary solar fuels research awards for the Fuels from Sunlight Hub program build on the unique accomplishments of the first Fuels from Sunlight Hub and address both new directions and long-standing challenges in the use of solar energy, water, and carbon dioxide as the only inputs for fuels production for clean energy. The FY 2022 Request will continue support for these early-stage fundamental research efforts that target innovative solutions to key scientific challenges for solar fuels (as identified in the strategic planning report from the Roundtable on Liquid Solar Fuels), including how to overcome degradation mechanisms to increase durability of solar fuel-generating components and systems, design catalytic microenvironments to selectively produce energy-rich solar fuels, take advantage of the direct coupling of light-driven phenomena and chemical processes to improve component and system performance, and tailor complex phenomena that interact and affect function of integrated multicomponent assemblies for solar fuels production.[a]

BES uses a variety of methods to regularly assess the progress of the awards, including annual progress reports, regular phone calls with the Directors, periodic Directors’ meetings to ensure coordination and communication, and on-site visits and reviews. Each award undergoes a review of its management structure and approach in the first year and beginning in the second year will have an annual peer review of research progress against its scientific goals.

[a] https://science.osti.gov/-/media/bes/pdf/reports/2020/Liquid_Solar_Fuels_Report.pdf

Computational Chemical Sciences

The computational chemical sciences program (CCS) supports basic research to develop validated, open-source codes and associated experimental/computational databases for modeling and simulation of complex chemical processes and phenomena that allow full use of emerging exascale and future planned DOE leadership-class computing capabilities. BES launched CCS research awards in FY 2017 and additional awards were initiated in FY 2018. The FY 2017 awards were recompeted in FY 2021. The FY 2018 awards will be recompeted in FY 2022. This research supports a publicly accessible website[a] of open source, robust, validated, user-friendly software that captures the essential physics and chemistry of relevant chemical systems. The goal is use of these codes/data by the broader research community and by industry to dramatically accelerate chemical research in the U.S.

BES uses a variety of methods to regularly assess the progress of the CCS awards, including annual progress reports, regular phone calls with the Directors, and periodic meetings of funded activities to ensure coordination and communication. Large team awards undergo a review of management structure and approach in the first year and a mid-term review by outside experts to evaluate scientific progress compared to the project's scientific goals.

General Plant Projects

GPP funding provides for minor new construction, for other capital alterations and additions, and for improvements to land, buildings, and utility systems to maintain the productivity and usefulness of DOE-owned facilities and to meet requirements for safe and reliable facilities operation.

[a] https://ccs-psi.org/

Activities and Explanation of Changes

(dollars in thousands)

FY 2021 Enacted		FY 2022 Request	Explanation of Changes FY 2022 Request vs FY 2021 Enacted
Chemical Sciences, Geosciences, and Biosciences	**$394,285**	**$448,939**	**+$54,654**
Fundamental Interactions Research	$107,904	$124,415	+$16,511
Funding continues to develop forefront ultrafast approaches, with emphasis on the use of x-ray free electron lasers, including LCLS and its upgrades. Gas-phase research continues studies of how reactive intermediates in heterogeneous environments impact reaction pathways, and quantum phenomena underlying QIS in tailored molecules. Research extends efforts to understand and control chemical processes and quantum phenomena at the molecular level in increasingly complex aqueous and interfacial systems. Research to understand and control interfacial chemical reactions increases with the aim of understanding the energy and chemical conversion mechanisms for clean-energy applications and of designing and synthesizing new materials relevant to microelectronics. This activity continues to develop advanced theoretical and computational approaches that can be scaled to operate on exascale computers. Development of AI/ML methods increases to enable novel data science approaches for knowledge discovery. Research emphasizes efforts to drive advances in the application of quantum information science for understanding and exploiting quantum phenomena in chemical systems. This activity provides continuing support for the QIS Research Centers established in FY 2020.		The Request will continue to develop forefront ultrafast approaches, with emphasis on the use of x-ray free electron lasers, including LCLS and its upgrades. Gas-phase research will continue studies of how reactive intermediates impact reaction pathways. Increased emphasis will be placed on quantum phenomena underlying QIS, such as coherence and entanglement. Research will extend efforts to understand and control chemical processes and quantum phenomena at the molecular level. Research to understand and control interfacial chemical reactions will continue with the aim of understanding the energy and chemical conversion mechanisms for clean-energy applications and of designing and synthesizing new materials relevant to microelectronics. This activity will continue to develop advanced theoretical and computational approaches that can be scaled to operate on exascale computers. Development of data science methods will increase to enable novel approaches for knowledge discovery. This activity provides continued support for the QIS Research Centers established in FY 2020.	Technical emphasis will include new efforts to unravel the fundamental mechanisms of energy and chemical conversions underlying clean-energy applications, to understand and exploit quantum phenomena important for QIS, and to understand and control interfacial chemical reactions that can enable new materials for microelectronics. Support will continue for the development of advanced theoretical and computational approaches, with focus on integration of data science and computational chemistry tools for the generation of scientific knowledge that is foundational to the BES mission. Expanded investment will include a focus on clean energy research in underrepresented communities and institutions.

(dollars in thousands)

FY 2021 Enacted		FY 2022 Request	Explanation of Changes FY 2022 Request vs FY 2021 Enacted
Chemical Transformations Research	$112,292	$117,725	+$5,433
Funding continues support for fundamental research to understand mechanisms of catalysis and to predict, design, and synthesize novel catalysts and bioinspired metal complexes with enhanced performance for thermo- and electro-chemical conversions important in clean-energy applications and chemical upcycling of polymers. Separation science research continues to focus on novel approaches to separate complex chemical mixtures with high efficiency, with increased focus on separation of carbon dioxide from dilute mixtures. Geosciences research continues to elucidate subsurface phenomena, such as mineral nucleation, and rock fracture propagation, with an emphasis on the intersection of geochemical and geophysical processes under extreme subsurface conditions. Heavy element research continues to deepen understanding of actinide speciation and reactivity, fundamental theories of f-electron systems, and approaches to synthesize and separate actinide compounds. Research on the chemistry of rare earth elements, including heavy elements such as lanthanides, focuses on understanding their reactivity to limit their use in catalytic processes, their interactions and chemical processes in multiphase systems relevant to separations, and their behavior in rare-earth containing minerals that are relevant to extraction in geological environments.		The Request will continue supporting fundamental research to understand catalytic mechanisms for thermo- and electro-chemical conversions important in clean-energy applications. Separation science research will continue to focus on innovative separation mechanisms for high-efficiency processes, including reactive and electro-separations, and novel solvents. Heavy element research will continue to deepen understanding of actinide speciation and reactivity and fundamental theories of f-electron systems. Geosciences research will continue to elucidate subsurface phenomena, such as mineralization and rock fracture propagation under extreme subsurface conditions. Areas for increased emphasis in FY 2022 include advances in atomically precise synthesis of new catalysts and in chemical processes that will gain the knowledge required to develop transformative, sustainable approaches in advanced manufacturing, such as combined catalysis and separations research for chemical upcycling of polymers; understanding of multiscale phenomena in extreme and constrained environments in the subsurface; and research on rare earth elements focused on advanced approaches to separations from complex and dilute mixtures, and discovery of alternative approaches that reduce their use.	Funding will emphasize research on catalysis and separation science research to provide the foundational knowledge needed for advanced manufacturing, including chemical upcycling of polymers, and microelectronics; for studies of the chemistry of rare earth and platinum-group elements important in critical materials to enable their improved separation, substitution, and reduction in use; and for development of innovative approaches to sustainable carbon and hydrogen cycles. The use of data science and AI/ML approaches will continue to be emphasized in research across the portfolio to accelerate the generation and sharing of scientific knowledge and its impact in clean-energy technologies. Expanded investment will include a focus on clean energy research in underrepresented communities and institutions.

(dollars in thousands)

FY 2021 Enacted		FY 2022 Request	Explanation of Changes FY 2022 Request vs FY 2021 Enacted
Photochemistry and Biochemistry Research	$82,589	$106,871	+$24,282
Funding continues to support fundamental research that emphasizes an understanding of the physical, chemical, and biochemical processes of light energy capture and conversion in biological and chemical systems. Studies of light absorption, energy transfer, charge transport and separation, separations processes, and photocatalysis in both natural and artificial systems provide fundamental knowledge to guide the design of new clean-energy systems. Funding increases focus on biochemical processes and complex structures that can enable development of bio-inspired, biohybrid, and biomimetic energy systems with desired functions and properties. Research on molecular mechanisms of biocatalysis, revealed by studies of enzyme structure and function, multi-electron redox reactions, and electron bifurcation, informs bioinspired design of catalysts and reaction pathways, for instance to guide new approaches for clean-energy applications and polymer upcycling. Research on metal uptake and use by biological systems informs bio-inspired separation processes. Studies also increase understanding of how rare elements can be minimized in photo-absorbers and catalysts for solar fuels. Advances in solar fuels continue via research on molecular mechanisms of photon capture, electron transfer, and product selectivity and separation from non-target molecules. Studies of light energy capture address the relationship between quantum phenomena and the efficiency and fidelity of energy transfer and conversion.		The Request will continue support of core research to understand physical, chemical, biophysical, and biochemical processes of light energy capture and conversion in biological and chemical systems. Studies of light absorption, energy transfer, charge transport, separation processes, and photocatalysis in natural and artificial systems will provide fundamental insights that can lead to innovations in the design of new clean-energy systems and processes. Knowledge of the molecular mechanisms of biocatalysis will guide the bio-inspired design of efficient catalysts and reaction pathways. Study of biochemical processes and structures will provide a foundation for bio-inspired, biohybrid, and biomimetic systems with desired functions and properties. Solar fuels research will continue to address the molecular mechanisms of photon capture, charge transport, product selectivity and separation from non-target molecules, and the reduction of rare elements and critical material use in photoabsorbers and catalysts. Biological and chemical studies will discover how quantum phenomena affect energy conversion efficiency and fidelity.	Technical emphasis will include research that targets fundamental science for innovation in advanced manufacturing, microelectronics, and clean-energy technologies through advances in fundamental biochemical, chemical, and biophysical principles; bio-inspired design and development of biomimetic and biohybrid energy systems and processes; and the discovery and understanding of mechanisms and processes of energy capture and conversion in both natural and artificial systems. Expanded investment will include a focus on clean energy research in underrepresented communities and institutions.

(dollars in thousands)

FY 2021 Enacted		FY 2022 Request	Explanation of Changes FY 2022 Request vs FY 2021 Enacted
Energy Frontier Research Centers	$57,500	$64,678	+$7,178
Funding provides the fourth year of support for four-year EFRC awards that were made in FY 2018 and the second year of support for four-year EFRC awards that were made in FY 2020.		The Request will provide the third year of support for four-year EFRC awards that were made in FY 2020 in the following topical areas: environmental management, polymer upcycling, and QIS. In addition, BES plans to issue a solicitation in FY 2022 to re-compete the EFRC awards made in FY 2018, with an emphasis on clean energy topics and other program priorities.	Technical emphasis for the EFRC program will include research directions identified in recent strategic planning activities. Expanded investment will include a focus on clean energy research in underrepresented communities and institutions.
Energy Innovation Hubs	$20,000	$20,758	+$758
Funding continues to support early-stage fundamental research on solar fuels generation to address both emerging new directions and long-standing scientific challenges in this area of energy science. Research continues to focus on generating fuels using only sunlight, carbon dioxide, and water as inputs. However, photodriven generation of fuels from molecules other than carbon dioxide can also provide important new insights into principles for solar energy capture and conversion into liquid fuels. Efforts that integrate experiment and theory and couple high-throughput experimentation with artificial intelligence continue to be emphasized.		The Request will continue support of early-stage fundamental research to address both long-standing and emerging new scientific challenges for solar fuels generation. Research will continue to focus on innovative artificial photosynthesis approaches to generate liquid fuels using only sunlight, carbon dioxide, and water as inputs. Experiment and theory are integrated for the design of processes, components, and systems for selective, stable, and efficient liquid solar fuels production for clean energy.	Funding will support priority research areas.

(dollars in thousands)

FY 2021 Enacted		FY 2022 Request	Explanation of Changes FY 2022 Request vs FY 2021 Enacted
Computational Chemical Sciences	$13,000	$13,492	+$492
Funding continues CCS awards made in FY 2018, with ongoing focus on developing public, open-source codes for future exascale computer platforms. In addition, FY 2021 funds support a recompetition of CCS awards made in FY 2017, and make awards for development of new theoretical and computational approaches and open-source codes in areas relevant to directions identified in BES strategic planning workshop reports.		The Request will continue CCS awards made in FY 2021, with ongoing focus on developing public, open-source codes for future exascale computer platforms. In addition, FY 2022 funds will support a recompetition of CCS awards made in FY 2018 and will make awards for development of new theoretical and computational approaches and open-source codes and databases in areas relevant to directions identified in BES strategic planning workshop reports.	Funding will support priority research areas for CCS awards as identified in BES strategic planning workshop reports. New investments will include a focus on clean energy research in underrepresented communities and institutions.
General Plant Projects	$1,000	$1,000	$ —
Funding supports minor facility improvements at Ames Laboratory.		The Request will support minor facility improvements at Ames Laboratory.	No changes.

Note: Funding for the subprogram above, includes 3.65% of research and development (R&D) funding for the Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) Programs.

Basic Energy Sciences
Scientific User Facilities (SUF)

Description

The Scientific User Facilities subprogram supports the operation of a geographically diverse suite of major research facilities that provide unique tools to thousands of researchers from a wide diversity of universities, industry, and government laboratories to advance a broad 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, researchers must use probes such as electrons, x-rays, 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 facilities, 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 with improved computational and data analysis infrastructure, improved nanoscience 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. Keeping BES accelerator-based facilities at the forefront requires continued, transformative advances in accelerator science and technology. Strategic investments in high-brightness electron injectors, superconducting undulators with strong focusing, and high gradient superconducting cavities will have the most impactful benefits. X-ray free electron laser (FEL) oscillators offer the most near-future attainable advances in x-ray science capabilities, requiring additional research efforts in x-ray resonant cavities and high heat-load diamond materials. Research in seeded FEL schemes for full coherent x-rays, and attosecond electron and x-ray pulse generation are critical for multi-terawatt FEL amplifiers required by single-particle imaging.

The twelve BES scientific user facilities provide the nation with the most comprehensive and advanced x-ray, neutron, and electron-based experimental tools enabling fundamental discovery science. Hundreds of experiments are conducted simultaneously around the clock, generating vast quantities of raw experimental data that must be stored, transported, and then analyzed to convert the raw data into information to unlock the answers to important scientific questions. Managing the collection, transport, and analysis of data at the BES facilities is a growing challenge as new facilities come online with expanded scientific capabilities coupled together with advances in detector technology. Over the next decade, the data volume, and the computational power to process the data, is expected to grow by several orders of magnitude. Applications of data science methods and tools are being implemented in new software and hardware to help address these data and information challenges and needs. Challenges include speeding up high-fidelity simulations for online models, fast tuning in high-dimensional space, anomaly/breakout detection, 'virtual diagnostics' that can operate at high repetition rates, and sophisticated compression/rejection data pipelines operating at the 'edge' (next to the instrument) to save the highest-value data from user experiments.

The BES user 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 to spin-based electronics and new drugs and delivery systems 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.

In FY 2019, more than 16,000 scientists and engineers in many fields of science and technology used BES scientific facilities. Due to the COVID-19 pandemic, BES scientific user facilities were under curtailed user operations, available mainly through remote access for the majority of the instruments during the second half of FY 2020. Additional funds provided through the CARES Act supported extraordinary operations of the light and neutron sources and nanoscale science research centers for COVID-specific research during curtailed operations. Light sources and neutron sources were able to provide critical support to the development of potential therapeutic drugs and vaccines through structural studies of the proteins of the SARS CoV-2 virus, which causes COVID-19. The BES facilities stand ready to continue to support ongoing research efforts to combat COVID-19 and future public health challenges. In FY 2022, continued support for biological threats at the light and neutron sources is recognized by the BRaVE initiative.

X-Ray Light Sources

X-rays are an essential tool for studying the structure of matter and have long been used to peer into material through which visible light cannot penetrate. Today's 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 desired behaviors. To this end, x-rays have become a primary tool for probing the atomic and electronic structure of materials internally and on their surfaces.

From their first systematic use as an experimental tool in the 1960s, large-scale light source facilities have vastly enhanced the utility of pre-existing and contemporary techniques, such as x-ray diffraction, x-ray spectroscopy, and imaging and have 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 x-ray light sources an important tool 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, and four storage ring-based light sources—the Advanced Light Source (ALS) at LBNL, the Advanced Photon Source (APS) at ANL, the Stanford Synchrotron Radiation Lightsource (SSRL) at SLAC, and the National Synchrotron Light Source-II (NSLS-II) at BNL. BES provides funds to support facility operations, to enable cutting-edge research and technical support, and to administer the user program at these facilities, which are made available to all researchers with access determined via peer review of user proposals.

Since completing construction of NSLS-II in FY 2015, BES has invested in the scientific research capabilities at this advanced light source facility by building specialized experimental stations or "beamlines." The initial suite of seven beamlines has expanded to the current 28 beamlines with room for at least 30 more. In order to adopt the most up-to-date technologies and to provide the most advanced capabilities, BES plans a phased approach to new beamlines at NSLS-II, as was done for the other light sources in the BES portfolio. The NSLS-II Experimental Tools-II (NEXT-II) major item of equipment (MIE) project was started in FY 2020 to provide three best-in-class beamlines to support the needs of the U.S. research community. These beamlines will focus on the techniques of coherent diffraction imaging, soft x-ray spectromicroscopy, and nanoscale probes of electronic excitations.

High-Flux Neutron Sources

One of the goals of modern materials science is to understand the factors that determine the properties of matter on the atomic scale and to use this knowledge to optimize those properties or to develop new materials and functionality. This process regularly involves the discovery of fascinating new physics, which itself may lead to previously unexpected applications. Among the different probes used to investigate atomic-scale structure and dynamics, 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 uniquely distinguished via isotope substitution experiments, for example substitution of deuterium for hydrogen 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 ORNL generates neutrons via fission in a research reactor. HFIR operates at 85 megawatts and provides state-of-the-art facilities for neutron scattering, isotope production, 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 instruments for inelastic scattering, small angle scattering, powder and single crystal diffraction, neutron imaging, and engineering diffraction.

The Spallation Neutron Source (SNS) at ORNL uses a different approach for generating neutron beams, where an accelerator generates protons that strike a heavy-metal target such as mercury. As a result of the impact, cascades of neutrons are produced in a process known as spallation.

The SNS is the world's brightest pulsed neutron facility, and presently includes 19 instruments. These world-leading instruments include very high-resolution inelastic and quasi-elastic scattering capabilities, powder and single crystal diffraction, polarized and unpolarized beam reflectometry, and spin echo and small angle scattering spectrometers. A large suite of capabilities for high and low temperature, high magnetic field, and high-pressure sample environment equipment is available for the instruments. All the SNS instruments are in high demand by researchers world-wide in a range of disciplines from biology to materials sciences and condensed matter physics.

Nanoscale Science Research Centers

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 while they interact with their physical and chemical environments. 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 Nanoscale Science Research Centers (NSRCs) focus on interdisciplinary discovery research at the nanoscale, serving as the basis for a national program that encompasses new science, new tools, and new computing capabilities. Distinct from the x-ray and neutron sources, NSRCs comprise of a suite of smaller unique tools and expert scientific staff. The five NSRCs are the Center for Nanoscale Materials at ANL, the Center for Functional Nanomaterials at BNL, the Molecular Foundry at LBNL, the Center for Nanophase Materials Sciences at ORNL, and the 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 and scanning probe microscopy; and nanostructure fabrication and integration. Selected thematic areas include catalysis, electronic materials, nanoscale photonics, and soft and biological materials. The centers are typically near BES facilities for x-rays or neutrons, or near SC-supported computation facilities, which complement and leverage each other's capabilities. These custom-designed laboratories contain clean rooms, nanofabrication resources, one-of-a-kind signature instruments, and other instruments generally available only at major user facilities. The NSRC electron and scanning probe microscopy capabilities provide superior atomic-scale spatial resolution and simultaneously obtain structural, chemical, and other types of information from sub-nanometer regions at short time scales. They house one of the highest resolution electron microscopes in the world. Data science approaches are enabling large and fast data acquisition, real-time analysis, and autonomous experiments. Operating funds enable cutting-edge research, provide technical support, and administer the user program at these facilities, which serve academic, government, and industry researchers with access determined through external peer review of user proposals.

The NSRCs will continue to develop nanoscience and QIS-related research infrastructure and capabilities for materials synthesis, device fabrication, metrology, modeling, and simulation. The goal is to develop a flexible and enabling infrastructure so that U.S. institutions and industry can rapidly develop and commercialize the new discoveries and innovations.

Other Project Costs

The total project cost (TPC) of DOE's construction projects comprises two major components—the total estimated cost (TEC) and other project costs (OPC). The TEC includes project costs incurred after Critical Decision-1, such as costs associated with all engineering design and inspection; the acquisition of land and land rights; direct and indirect construction/fabrication; 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, such as costs that are incurred during the project's initiation and definition phase for planning, conceptual design, research, and development, and those incurred during the execution phase for R&D, startup, and commissioning. OPC is always funded via operating funds.

Major Items of Equipment

BES supports major item of equipment (MIE) projects to ensure the continual development and upgrade of major scientific instrument capabilities, including fabricating new x-ray and neutron experimental stations, improving NSRC core facilities, and providing new stand-alone instruments and capabilities.

Research

This activity supports targeted basic research in accelerator physics, x-ray and neutron detectors, and development of advanced x-ray optics that is specific to BES facility needs and directions. BES coordinates with the SC Office of Accelerator R&D and Production on crosscutting research and technology areas. Accelerator research is the cornerstone for the development of new technologies that will improve performance of accelerator-based light sources and neutron scattering facilities, in support of the Accelerator Science and Technology Initiative. Research areas include ultrashort pulse free electron lasers (FELs), new seeding techniques and other optical manipulations to reduce the cost and complexity and improve performance of next-generation FELs, and development of intense laser-based terahertz (THz) sources to study non-equilibrium behavior in complex materials. As the complexity of accelerators and the performance requirements continue to grow the need for more dynamic and adaptive control systems becomes essential. Particle accelerators are complicated interconnected machines and ideal for applications of the most advanced Artificial Intelligence (AI)/Machine Learning (ML) algorithms to improve performance optimization, rapid recovery of fault conditions, and prognostics to anticipate problems. Detector research is a crucial component to enable the optimal utilization of BES 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 supports training in the field of particle beams and their associated accelerator applications.

Activities and Explanation of Changes

(dollars in thousands)

FY 2021 Enacted		FY 2022 Request	Explanation of Changes FY 2022 Request vs FY 2021 Enacted
Scientific User Facilities (SUF)	**$1,026,707**	**$1,057,200**	**+$30,493**
X-Ray Light Sources	$525,000	$538,282	+$13,282
The funding supports operations at five BES light sources (LCLS, APS, ALS, NSLS-II, and SSRL).		The Request will support operations at five BES light sources (LCLS, APS, ALS, NSLS-II, and SSRL).	Funding will support LCLS, APS, ALS, NSLS-II and SSRL operations at 97 percent of optimal.
High-Flux Neutron Sources	$292,000	$293,871	+$1,871
The funding supports operations at SNS and HFIR.		The Request will support operations at SNS and HFIR.	Funding will support operations for SNS and HFIR at approximately 96 percent of optimal.
Nanoscale Science Research Centers	$139,000	$142,387	+$3,387
The funding supports operations for the five NSRCs (CFN, CNM, CNMS, TMF, and CINT). The NSRCs continue to develop nanoscience and QIS-related research infrastructure and capabilities for materials synthesis, device fabrication, metrology, modeling and simulation.		The Request will provide funding for five NSRCs (CFN, CNM, CNMS, TMF, and CINT). The NSRCs will continue to develop nanoscience and QIS-related research infrastructure and capabilities for materials synthesis, device fabrication, metrology, modeling and simulation.	Funding will support operations for the five NSRCs at 96 percent of optimal, including support to develop QIS-related research infrastructure and capabilities.
Other Project Costs	$19,000	$14,300	-$4,700
Other Project Costs continue for the LCLS-II-HE project at SLAC National Accelerator Laboratory, PPU at Oak Ridge National Laboratory, Second Target Station project at Oak Ridge National Laboratory, and the Cryomodule Repair and Maintenance Facility (CRMF) project at SLAC.		The Request will support Other Project Costs for the LCLS-II-HE project at SLAC National Accelerator Laboratory, PPU at Oak Ridge National Laboratory, the Second Target Station project at Oak Ridge National Laboratory, and the Cryomodule Repair and Maintenance Facility (CRMF) project at SLAC.	Other Project Costs follow project plans.

(dollars in thousands)

FY 2021 Enacted		FY 2022 Request	Explanation of Changes FY 2022 Request vs FY 2021 Enacted
Major Items of Equipment	$10,500	$30,000	+$19,500
The funding supports the beamline project for NSLS-II (NEXT-II) at Brookhaven National Laboratory. Design work for NEXT-II will continue along with R&D, prototyping, other supporting activities, and possible long lead procurements. The recapitalization project for the NSRCs also continues with R&D, design, engineering, prototyping, other supporting activities, and possible procurements. The project received CD-1/3A approval on 4/15/2021.		The Request will continue the beamline project for NSLS-II (NEXT-II) at Brookhaven National Laboratory. Design work for NEXT-II will continue along with R&D, prototyping, other supporting activities, long lead procurements and construction/equipment procurements. The project is planning for CD-2/3 approval early in FY 2022. The recapitalization project for the NSRCs will also continue with R&D, design, engineering, prototyping, other supporting activities, and possibly long-lead procurements. The project is planning for CD-2/3 approval in FY 2022.	Funding will support the NEXT-II and NSRC Recapitalization MIE projects.
Research	$41,207	$38,360	-$2,847
The funding supports high-priority research activities for advanced seeded FEL schemes that provide several orders of magnitude performance enhancement, detectors and optics instrumentation and applications of machine learning techniques to accelerator optimization, control, prognostics, and data analysis. Research will emphasize transformative advances in accelerator science and technology that lead to significant improvements in very high brightness and high current electron sources and in high intensity proton sources.		The Request will support high-priority research activities for advanced seeded FEL schemes that provide several orders of magnitude performance enhancement, detectors with high read out rate, optics that can handle high heat load and preserve the coherent wave front, and applications of data science techniques to accelerator optimization, control, prognostics, and data analysis. Research will emphasize transformative advances in accelerator science and technology that lead to significant improvements in very high brightness and high current electron sources and in high intensity proton sources.	Funding will support investment in future accelerator technologies to continue to provide the world's most comprehensive and advanced accelerator-based facilities for scientific research. Funding will also continue the development of data science methods and tools to address data and information challenges at the BES user facilities, including accelerator optimization, control, prognostics, and experiment automation and real time data analysis.

Note: Funding for the subprogram above, includes 3.65% of research and development (R&D) funding for the Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) Programs.

Basic Energy Sciences
Construction

Description

Accelerator-based x-ray light sources, accelerator-based pulsed neutron sources, and reactor-based neutron sources are essential user facilities that enable critical DOE mission-driven science, including research in support of clean energy, as well as research in response to national priorities such as the COVID-19 pandemic. 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.

<u>21-SC-10, Cryomodule Repair & Maintenance Facility (CRMF), SLAC</u>

The CRMF project will provide a much needed capability to maintain, repair, and test superconducting radiofrequency (SRF) accelerator components. These components include but are not limited to superconducting RF cavities and cryomodules that make up the new superconducting accelerator being constructed by the LCLS-II and LCLS-II-HE projects, high brightness electron injectors, and superconducting undulators. The facility will provide for the full disassembly and repair of the SRF cryomodule; the ability to disassemble, clean, and reassemble the SRF cavities and cavity string; testing capabilities for the full cryomodule; and separate testing capabilities for individual SRF cavities. To accomplish this, the project is envisioned to require a 19,000 to 23,000 gross square foot building to contain the necessary equipment. The building will need a concrete shielded enclosure for cryomodule testing, a control room, vertical test stand area for testing SRF cavities and components, a cryogen distribution box which is connected to a source of liquid helium and will distribute liquid helium within the CRMF building, cryomodule fixtures used to insert and remove the cold mass from the cryomodule vacuum vessel, a cleanroom partitioned into class 10 and class 1000 areas, a loading and cryomodule preparation area, storage areas, and a 15 ton bridge crane for moving equipment from one area to another within the building. The project received CD-0, Approve Mission Need, on December 5, 2019. The current TPC range is $70,000,000–$98,000,000.

<u>19-SC-14, Second Target Station (STS), ORNL</u>

The STS project will expand SNS capabilities for neutron scattering research by exploiting part of the higher SNS accelerator proton beam power (2.8 MW) enabled by the PPU project. The STS will be a complementary pulsed source with a narrow proton beam which increases the proton beam power density compared to the first target station (FTS). This dense beam of protons, when deposited on a compact, rotating, water-cooled tungsten target, will create neutrons through spallation and direct them to high efficiency coupled moderators to produce an order of magnitude higher brightness cold neutrons than were previously achievable. By optimizing the design of the instruments with advanced neutron optics, optimized geometry for 15 Hz operation, and advanced detectors, the detection resolution will be up to two orders of magnitude higher, enabling new research opportunities. The project received CD-1, Approve Alternative Selection and Cost Range, on November 23, 2020, which established the approved TPC range of $1,800,000,000–$3,000,000,000.

<u>18-SC-10, Advanced Photon Source Upgrade (APS-U), ANL</u>

The APS-U project will 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 x-ray brightness and coherent flux. Nine new x-ray beamlines will be installed and several existing beamlines will be upgraded to take advantage of the enhanced x-ray properties. APS-U will ensure that the APS remains a world leader in hard x-ray science. The project received approval for CD-3, Approve Start of Construction, on July 25, 2019, with a Total Project Cost (TPC) of $815,000,000 and CD-4, Approve Project Completion, projected in 2Q FY 2026.

<u>18-SC-11, Spallation Neutron Source Proton Power Upgrade (PPU), ORNL</u>

The PPU project will double the proton beam power capability of the Spallation Neutron Source (SNS) from 1.4 megawatts (MW) to 2.8 MW by fabricating and installing seven new superconducting radio frequency (SRF) cryomodules and supporting RF equipment, upgrade the first target station to accommodate beam power up to 2 MW, and deliver a 2 MW-qualified target. The high voltage converter modulators and klystrons for some of the existing installed RF equipment will be upgraded to handle the higher beam current. The accumulator ring will be upgraded with minor modifications to the injection and extraction areas. The improved target performance at the increased beam power of 2 MW is enabled by the addition of a new gas injection system and a redesigned mercury target vessel. The project received CD-3, Approve Start of Construction, on October 6, 2020, with a Total Project Cost (TPC) of $271,567,000 and CD-4, Approve Project Completion, expected in 4Q FY 2028.

18-SC-12, Advanced Light Source Upgrade (ALS-U), LBNL
The ALS-U project will upgrade the existing ALS facility by replacing the existing electron storage ring with a new electron storage ring based on a multi-bend achromat lattice design, which will provide a soft x-ray source that is up to 1000 times brighter and with a significantly higher coherent flux fraction. ALS-U will leverage two decades of investments in scientific tools at the ALS by making use of the existing beamlines and infrastructure. ALS-U will ensure that the ALS facility remains a world leader in soft x-ray science. The project received CD-3A, Approve Long Lead Procurements, on December 19, 2019. The project received CD-2, Approve Performance Baseline, on April 2, 2021. The project CD-2 Total Project Cost (TPC) is $590,000,000 with a projected CD-3, Approve Start of Construction, in 3Q of FY 2022.

18-SC-13, Linac Coherent Light Source-II-High Energy (LCLS-II-HE), SLAC
The LCLS-II-HE project will increase the energy of the superconducting linac currently under construction as part of the LCLS-II project from 4 giga-electronvolts (GeV) to 8 GeV and thereby expand the high repetition rate operation (1 million pulses per second) of this unique facility into the hard x-ray regime (5-12 keV). LCLS-II-HE will add new and upgraded instrumentation to augment existing capabilities and upgrade the facility infrastructure as needed. The LCLS-II-HE project will upgrade and expand the capabilities of the LCLS-II to maintain U.S. leadership in ultrafast x-ray science. The project received CD-3A, Approve Long Lead Procurements, on May 12, 2020, with the TPC range of $290,000,000–$480,000,000. Between CD-3A and the current budget process, the TPC estimate has increased to $660,000,000 as a result of a maturing design effort that identified additional costs across the project scope, added scope for a new superconducting electron source, and increased the project's contingency to address several future risks. The LCLS-II-HE project is currently assessing the impact of COVID-19 on the project's cost and schedule. The key milestones have been delayed and the combined CD-2/3 approval is now projected for 4Q FY 2022 and CD-4 now projected for 2Q FY 2030.

13-SC-10, Linac Coherent Light Source II (LCLS-II), SLAC
The LCLS-II project will provide a second source of electrons at LCLS by constructing a 4 GeV, high repetition rate, superconducting linear accelerator in addition to adding two new variable gap undulators to generate an unprecedented high-repetition-rate free-electron laser. This new x-ray source will solidify the LCLS complex as the world leader in ultrafast x-ray science for decades to come. The project received approval for CD-2, Approve Performance Baseline, and CD-3, Approve Start of Construction, on March 21, 2016, establishing a Total Project Cost (TPC) of $1,045,000,000 and a CD-4, Project Completion date of June 30, 2022. Due largely to COVID impacts, the project suffered a Baseline Deviation in FY 2020. The Baseline Change Proposal was approved on October 13, 2020, establishing a new TPC of $1,136,400,000 and a new CD-4 date of January 2024.

All BES construction projects are conceived and planned with the scientific community, 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 percent of the cost and schedule performance baselines, established at CD-2, Approve Performance Baseline, which are reproduced in the construction project data sheets.

Activities and Explanation of Changes

(dollars in thousands)

FY 2021 Enacted		FY 2022 Request	Explanation of Changes FY 2022 Request vs FY 2021 Enacted
Construction	**$389,000**	**$304,200**	**-$84,800**
21-SC-10, Cryomodule Repair & Maintenance Facility (CRMF), SLAC	$1,000	$1,000	$ —
Funding supports conducting a conceptual design and an Analysis of Alternatives to determine a revised cost range for the project at SLAC. Engineering and design activities may begin.		The FY 2022 Request will continue to support the conceptual design effort and possibly the initial engineering design work depending on progress and CD approvals.	Funding will advance progress on the CRMF project.
19-SC-14, Second Target Station (STS), ORNL	$29,000	$32,000	+$3,000
Funding continues to support planning, R&D, and engineering activities to assist in maturing the project preliminary design, scope, cost, schedule and key performance parameters with emphasis on advancing the accelerator, target, instrument, controls, and conventional civil construction subsystems.		In FY 2022, the project will continue the FY 2021 activities of planning, R&D, and engineering to assist in maturing the project preliminary design, scope, cost, schedule and key performance parameters with continued emphasis on advancing the accelerator, target, instrument, controls, and conventional civil construction subsystems.	Funding will advance progress on the STS project.

(dollars in thousands)

FY 2021 Enacted		FY 2022 Request	Explanation of Changes FY 2022 Request vs FY 2021 Enacted
18-SC-10, Advanced Photon Source Upgrade (APS-U), ANL	$160,000	$101,000	-$59,000
Funding continues to support advancing the final designs, engineering, prototyping, testing, fabrication, procurement of baseline and spare hardware, integration, and installation for the storage ring and experimental facilities, and site preparation and civil construction associated with the long beamlines.		The FY 2022 Request will support ongoing activities to advance the final designs, engineering, prototyping, testing, fabrication, procurement of baseline and spare hardware, integration, and installation for the storage ring and experimental facilities. Further civil construction associated with the long beamline building will occur. System integration, test, and assembly in preparation for the storage ring removal and installation during the experimental dark time will be a high priority.	Funding will advance progress on the APS-U project. The APS-U current baseline (from the CD-2 approval) does not include potential COVID impacts that could increase the baseline cost and extend the schedule; this situation is being carefully monitored.
18-SC-11, Spallation Neutron Source Proton Power Upgrade (PPU), ORNL	$52,000	$17,000	-$35,000
Funding continues to support R&D, engineering, prototyping, design, testing, fabrication, procurement of baseline and spare hardware, component integration and installation, and civil construction. Advancing the target R&D, engineering, design, and prototyping in conjunction with SNS operations target improvement plans will be a high priority.		In FY 2022, the project will prioritize continuing activities of R&D, engineering, prototyping, design, testing, fabrication, procurement of baseline and spare hardware, component integration and installation, and civil construction site preparation with priority on continuing RF equipment installation in the klystron gallery, cryomodule assembly, first complete cryomodule receipt, and advancing the target knowledge base by running the first PPU test target during SNS operations.	Funding will advance progress on the PPU project.
18-SC-12, Advanced Light Source Upgrade (ALS-U), LBNL	$62,000	$75,100	+$13,100
Funding continues to support engineering, design, R&D prototyping and long lead procurements of construction items and other tasks as required.		Funding will continue support of engineering, design, R&D prototyping, and long lead procurements of construction items. Authorization of full construction activities is anticipated for early FY 2022.	Funding will advance progress on the ALS-U project.

(dollars in thousands)

FY 2021 Enacted		FY 2022 Request	Explanation of Changes FY 2022 Request vs FY 2021 Enacted
18-SC-13, Linac Coherent Light Source-II-High Energy (LCLS-II-HE), SLAC	$52,000	$50,000	-$2,000
Funding continues to support engineering, design, R&D prototyping, and long lead procurements of construction items as authorized along with other tasks as required.		Funding will support engineering, design, R&D prototyping, continuing long lead procurements of construction items and preparation of the project baseline. Other tasks as required.	Funding will advance progress on the LCLS-II-HE project.
13-SC-10 - Linac Coherent Light Source-II (LCLS-II), SLAC	$33,000	$28,100	-$4,900
Funding continues to support installation of all remaining major accelerator and x-ray systems and equipment commissioning activities.		Funding will be used to complete installation of any remaining major accelerator and x-ray systems and equipment commissioning activities.	Funding will support completion of the LCLS II project.

Basic Energy Sciences
Capital Summary

	(dollars in thousands)					
	Total	Prior Years	FY 2020 Enacted	FY 2021 Enacted	FY 2022 Request	FY 2022 Request vs FY 2021 Enacted
Capital Operating Expenses						
Capital Equipment	N/A	N/A	46,825	46,950	65,800	+18,850
Minor Construction Activities						
General Plant Projects	N/A	N/A	1,000	10,000	11,500	+1,500
Accelerator Improvement Projects	N/A	N/A	10,700	30,539	42,820	+12,281
Total, Capital Operating Expenses	**N/A**	**N/A**	**58,525**	**87,489**	**120,120**	**+32,631**

Capital Equipment

	(dollars in thousands)					
	Total	Prior Years	FY 2020 Enacted	FY 2021 Enacted	FY 2022 Request	FY 2022 Request vs FY 2021 Enacted
Capital Equipment						
Major Items of Equipment						
Scientific User Facilities (SUF)						
NSLS-II Experimental Tools-II (NEXT-II), BNL	94,500	–	5,500	5,500	15,000	+9,500
NSRC Recapitalization	80,000	–	5,000	5,000	15,000	+10,000
Total, MIEs	N/A	N/A	10,500	10,500	30,000	+19,500
Total, Non-MIE Capital Equipment	N/A	N/A	36,325	36,450	35,800	-650
Total, Capital Equipment	**N/A**	**N/A**	**46,825**	**46,950**	**65,800**	**+18,850**

Note: GPP activities less than $5M include design and construction for additions and/or improvements to land, buildings, replacements or addition to roads, and general area improvements. AIP activities less than $5M include minor construction at an existing accelerator facility.

Minor Construction Activities

(dollars in thousands)

	Total	Prior Years	FY 2020 Enacted	FY 2021 Enacted	FY 2022 Request	FY 2022 Request vs FY 2021 Enacted
General Plant Projects (GPP)						
GPPs (greater than or equal to $5M and less than $20M)						
HFIR Guide Hall Extension	18,000	–	–	9,000	9,000	–
Total GPPs (greater than or equal to $5M and less than $20M)	N/A	N/A	–	9,000	9,000	–
Total GPPs less than $5M	N/A	N/A	1,000	1,000	2,500	+1,500
Total, General Plant Projects (GPP)	**N/A**	**N/A**	**1,000**	**10,000**	**11,500**	**+1,500**
Accelerator Improvement Projects (AIP)						
AIPs (greater than or equal to $5M and less than $20M)						
Storage Ring HVAC System Upgrade, ALS	6,900	650	6,250	–	–	–
3rd Harmonic Cavity, NSLS-II	5,211	–	–	–	5,211	+5,211
Spallation Neutron Source Cold Box-Engineering	500	–	–	–	500	+500
Spare Cold Box for RF Cryoplant	5,200	–	–	5,200	–	-5,200
Cold Source Helium Refrigerator System	9,339	–	–	9,339	–	-9,339
Moderator Test Stand (SNS)	6,250	–	–	–	6,250	+6,250
160kW Solid State Amplifier Hardware and Utilities - Phase 2 (APS)	10,958	–	–	–	10,958	+10,958
Total AIPs (greater than or equal to $5M and less than $20M)	N/A	N/A	6,250	14,539	22,919	+8,380
Total AIPs less than $5M	N/A	N/A	4,450	16,000	19,901	+3,901
Total, Accelerator Improvement Projects (AIP)	**N/A**	**N/A**	**10,700**	**30,539**	**42,820**	**+12,281**
Total, Minor Construction Activities	**N/A**	**N/A**	**11,700**	**40,539**	**54,320**	**+13,781**

Basic Energy Sciences
Major Items of Equipment Description(s)

Scientific User Facilities (SUF) MIEs:

NSLS-II Experimental Tools-II (NEXT-II) Project

The NEXT-II project proposes to add three world-class beamlines to the NSLS-II Facility as part of a phased buildout of beamlines to provide advances in scientific capabilities for the soft x-ray user community. These beamlines will focus on the techniques of coherent diffraction imaging, soft x-ray spectromicroscopy, and nanoscale probes of electronic excitations. The project received CD-1, Approve Alternative Selection and Cost Range, on September 30, 2020. The CD-1 approved total project cost range is $65,000,000 to $95,000,000 with a point estimate of $89,000,000. The FY 2022 Request of $15,000,000 will continue R&D, prototyping, other supporting activities, and construction/equipment procurements. The project is planning for CD-2/3 approval early in FY 2022.

Nanoscale Science Research Center (NSRC) Recapitalization Project

The NSRCs started early operations in 2006-2007 and now, a decade later, instrumentation recapitalization is needed to continue to perform cutting edge science to support and accelerate advances in the fields of nanoscience, materials, chemistry, and biology. The recapitalization will also provide essential support for quantum information science and systems. The project received a combined CD-1, Approve Alternative Selection and Cost Range, and CD-3A, Approve Long-Lead Procurements, on April 15, 2021. The current total project cost range is $70,000,000 to $95,000,000 with a point estimate of $80,000,000. The FY 2022 Request of $15,000,000 will continue R&D, design, engineering, prototyping, other supporting activities, and construction/equipment procurements. The project is planning for CD-2/3 approval in FY 2022.

Basic Energy Sciences
Construction Projects Summary

(dollars in thousands)

	Total	Prior Years	FY 2020 Enacted	FY 2021 Enacted	FY 2022 Request	FY 2022 Request vs FY 2021 Enacted
21-SC-10, Cryomodule Repair & Maintenance Facility (CRMF), SLAC						
Total Estimated Cost (TEC)	88,000	–	–	1,000	1,000	–
Other Project Cost (OPC)	10,000	–	–	1,000	2,000	+1,000
Total Project Cost (TPC)	**98,000**	**–**	**–**	**2,000**	**3,000**	**+1,000**
19-SC-14, Second Target Station, ORNL						
Total Estimated Cost (TEC)	2,143,000	1,000	20,000	29,000	32,000	+3,000
Other Project Cost (OPC)	99,000	15,805	17,000	13,000	–	-13,000
Total Project Cost (TPC)	**2,242,000**	**16,805**	**37,000**	**42,000**	**32,000**	**-10,000**
18-SC-10, Advanced Photon Source Upgrade, ANL						
Total Estimated Cost (TEC)	796,500	363,300	170,000	160,000	101,000	-59,000
Other Project Cost (OPC)	18,500	8,500	–	–	5,000	+5,000
Total Project Cost (TPC)	**815,000**	**371,800**	**170,000**	**160,000**	**106,000**	**-54,000**
18-SC-11, Spallation Neutron Source Proton Power Upgrade, ORNL						
Total Estimated Cost (TEC)	257,802	96,000	60,000	52,000	17,000	-35,000
Other Project Cost (OPC)	13,798	10,798	–	3,000	–	-3,000
Total Project Cost (TPC)	**271,600**	**106,798**	**60,000**	**55,000**	**17,000**	**-38,000**
18-SC-12, Advanced Light Source Upgrade, LBNL						
Total Estimated Cost (TEC)	562,000	76,000	60,000	62,000	75,100	+13,100
Other Project Cost (OPC)	28,000	26,000	2,000	–	–	–
Total Project Cost (TPC)	**590,000**	**102,000**	**62,000**	**62,000**	**75,100**	**+13,100**

(dollars in thousands)

	Total	Prior Years	FY 2020 Enacted	FY 2021 Enacted	FY 2022 Request	FY 2022 Request vs FY 2021 Enacted
18-SC-13, Linac Coherent Light Source-II-High Energy, SLAC						
Total Estimated Cost (TEC)	644,543	33,200	50,000	52,000	50,000	-2,000
Other Project Cost (OPC)	32,000	8,000	4,000	2,000	3,000	+1,000
Total Project Cost (TPC)	**676,543**	**41,200**	**54,000**	**54,000**	**53,000**	**-1,000**
13-SC-10, Linac Coherent Light Source II (LCLS-II), SLAC						
Total Estimated Cost (TEC)	1,060,856	999,756	–	33,000	28,100	-4,900
Other Project Cost (OPC)	56,200	51,900	–	–	4,300	+4,300
Total Project Cost (TPC)	**1,117,056**	**1,051,656**	**–**	**33,000**	**32,400**	**-600**
Total, Construction						
Total Estimated Cost (TEC)	**N/A**	**N/A**	**360,000**	**389,000**	**304,200**	**-84,800**
Other Project Cost (OPC)	**N/A**	**N/A**	**23,000**	**19,000**	**14,300**	**-4,700**
Total Project Cost (TPC)	**N/A**	**N/A**	**383,000**	**408,000**	**318,500**	**-89,500**

Basic Energy Sciences
Funding Summary

(dollars in thousands)

	FY 2020 Enacted	FY 2021 Enacted	FY 2022 Request	FY 2022 Request vs FY 2021 Enacted
Research	871,321	869,500	975,960	+106,460
Facility Operations	947,179	956,000	974,540	+18,540
Projects				
Line Item Construction (LIC)	383,000	408,000	318,500	-89,500
Major Items of Equipment (MIE)	10,500	10,500	30,000	+19,500
Total, Projects	**393,500**	**418,500**	**348,500**	**-70,000**
Other	1,000	1,000	1,000	–
Total, Basic Energy Sciences	**2,213,000**	**2,245,000**	**2,300,000**	**+55,000**

Basic Energy Sciences
Scientific User Facility Operations

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 for TYPE A facilities:

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.

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.

	(dollars in thousands)				
	FY 2020 Enacted	**FY 2020 Current**	**FY 2021 Enacted**	**FY 2022 Request**	**FY 2022 Request vs FY 2021 Enacted**
Scientific User Facilities - Type A					
Advanced Light Source	**68,093**	**68,393**	**68,908**	**70,704**	**+1,796**
Number of Users	1,800	1,816	1,800	1,400	-400
Achieved Operating Hours	–	3,239	–	–	–
Planned Operating Hours	3,880	3,880	3,168	3,300	+132
Optimal Hours	3,880	–	4,100	3,400	-700
Percent of Optimal Hours	100.0%	83.5%	93.2%	97.1%	+3.9%
Advanced Photon Source	**140,477**	**140,627**	**142,158**	**146,226**	**+4,068**
Number of Users	4,900	4,323	4,300	4,000	-300
Achieved Operating Hours	–	5,436	–	–	–
Planned Operating Hours	5,000	5,000	5,000	3,980	-1,020
Optimal Hours	5,000	–	5,000	4,100	-900
Percent of Optimal Hours	100.0%	108.7%	100.0%	97.1%	-2.9%
National Synchrotron Light Source	**117,244**	**117,394**	**118,647**	**121,243**	**+2,596**
Number of Users	1,700	1,356	1,300	1,600	+300
Achieved Operating Hours	–	5,416	–	–	–
Planned Operating Hours	5,000	5,000	4,500	4,850	+350
Optimal Hours	5,000	–	5,000	5,000	–
Percent of Optimal Hours	100.0%	108.3%	93.8%	97.0%	+3.2%

(dollars in thousands)

	FY 2020 Enacted	FY 2020 Current	FY 2021 Enacted	FY 2022 Request	FY 2022 Request vs FY 2021 Enacted
Stanford Synchrotron Radiation Light Source	**44,017**	**44,167**	**44,544**	**46,447**	**+1,903**
Number of Users	1,500	963	950	1,350	+400
Achieved Operating Hours	–	4,467	–	–	–
Planned Operating Hours	5,090	5,090	5,020	5,050	+30
Optimal Hours	5,090	–	5,400	5,200	-200
Percent of Optimal Hours	100.0%	87.8%	93.0%	97.1%	+4.1%
Linac Coherent Light Source	**148,960**	**160,875**	**150,743**	**153,662**	**+2,919**
Number of Users	500	291	800	800	–
Achieved Operating Hours	–	705	–	–	–
Planned Operating Hours	2,800	2,500	4,500	4,560	+60
Optimal Hours	2,800	–	4,600	4,700	+100
Percent of Optimal Hours	100.0%	28.2%	97.8%	97.0%	-0.8%
Spallation Neutron Source	**187,048**	**182,638**	**183,532**	**185,081**	**+1,549**
Number of Users	800	611	730	800	+70
Achieved Operating Hours	–	4,829	–	–	–
Planned Operating Hours	4,600	4,600	4,600	4,350	-250
Optimal Hours	4,600	–	5,000	4,600	-400
Percent of Optimal Hours	100.0%	105.0%	93.9%	94.6%	+0.7%
High Flux Isotope Reactor	**102,653**	**107,579**	**108,468**	**108,790**	**+322**
Number of Users	520	280	500	560	+60
Achieved Operating Hours	–	3,631	–	–	–
Planned Operating Hours	3,900	3,900	3,100	3,900	+800
Optimal Hours	3,900	–	4,000	4,000	–
Percent of Optimal Hours	100.0%	93.1%	93.9%	97.5%	+3.6%

	(dollars in thousands)				
	FY 2020 Enacted	**FY 2020 Current**	**FY 2021 Enacted**	**FY 2022 Request**	**FY 2022 Request vs FY 2021 Enacted**
Scientific User Facilities - Type B					
Center for Nanoscale Materials	**28,461**	**28,562**	**28,275**	**28,555**	**+280**
Number of Users	530	484	500	480	-20
Center for Functional Nanomaterials	**24,807**	**24,907**	**25,113**	**26,864**	**+1,751**
Number of Users	510	546	500	520	+20
Molecular Foundry	**32,090**	**32,191**	**32,162**	**32,484**	**+322**
Number of Users	800	740	700	750	+50
Center for Nanophase Materials Sciences	**27,818**	**27,920**	**28,131**	**28,412**	**+281**
Number of Users	630	578	500	580	+80
Center for Integrated Nanotechnologies	**25,511**	**25,612**	**25,319**	**26,072**	**+753**
Number of Users	700	654	600	660	+60
Total, Facilities	**947,179**	**960,865**	**956,000**	**974,540**	**+18,540**
Number of Users	14,890	12,642	13,180	13,500	+320
Achieved Operating Hours	–	27,723	–	–	–
Planned Operating Hours	30,270	29,970	29,888	29,990	+102
Optimal Hours	30,270	–	33,100	31,000	-2,100

Note: Achieved Operating Hours and Unscheduled Downtime Hours will only be reflected in the Congressional budget cycle which provides actuals.

Basic Energy Sciences
Scientific Employment

	FY 2020 Enacted	FY 2021 Enacted	FY 2022 Request	FY 2022 Request vs FY 2021 Enacted
Number of Permanent Ph.Ds (FTEs)	4,950	4,860	5,370	+510
Number of Postdoctoral Associates (FTEs)	1,370	1,340	1,530	+190
Number of Graduate Students (FTEs)	2,140	2,090	2,420	+330
Number of Other Scientific Employment (FTEs)	3,100	3,050	3,250	+200

Note: Other Scientific Employment (FTEs) includes technicians, engineers, computer professionals and other support staff.

21-SC-10, Cryomodule Repair & Maintenance Facility (CRMF), SLAC
SLAC National Accelerator Laboratory
Project is for Design and Construction

1. Summary, Significant Changes, and Schedule and Cost History

Summary

The FY 2022 Request for the Cryomodule Repair and Maintenance Facility (CRMF) project at SLAC National Accelerator Laboratory is $1,000,000 of Total Estimated Cost (TEC) funding and $2,000,000 in Other Projects Costs (OPC) funding. This project has a preliminary Total Estimated Cost (TEC) range of $60,000,000 to $88,000,000 and a preliminary Total Project Cost (TPC) range of $70,000,000 to $98,000,000. These cost ranges encompass the most feasible preliminary alternatives at this time. The preliminary TPC estimate for this project is $98,000,000.

Significant Changes

CRMF was initiated in FY 2021. The most recent DOE Order 413.3B approved Critical Decision (CD) is CD-0, Approve Mission Need, approved on December 5, 2019.

In FY 2021, both a conceptual design for the facility and an Analysis of Alternatives (AoA) based on that conceptual design will be conducted to determine a revised cost range for the project. Engineering and design activities may begin. The FY 2022 Request will support ongoing activities to support the conceptual design effort and possibly the initial engineering design work depending on progress and CD approvals.

A Federal Project Director will be assigned to this project prior to CD-1 approval.

Critical Milestone History

Fiscal Year	CD-0	Conceptual Design Complete	CD-1	CD-2	Final Design Complete	CD-3	D&D Complete	CD-4
FY 2021	12/5/19	1Q FY 2021	1Q FY 2021	1Q FY 2022	4Q FY 2022	1Q FY 2023	N/A	1Q FY 2027
FY 2022	12/5/19	4Q FY 2022	4Q FY 2022	4Q FY 2023	2Q FY 2024	2Q FY 2024	N/A	4Q FY 2028

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 Alternative Selection and Cost Range
CD-2 – Approve 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

Fiscal Year	Performance Baseline Validation	CD-3A
FY 2021	4Q FY 2021	1Q FY 2022
FY 2022	4Q FY 2023	4Q FY 2023

CD-3A – Approve Long-Lead Procurements: As the project planning and design matures, long lead procurement may be requested to mitigate cost and schedule risk to the project.

Project Cost History

(dollars in thousands)

Fiscal Year	TEC, Design	TEC, Construction	TEC, Total	OPC, Except D&D	OPC, D&D	OPC, Total	TPC
FY 2021	4,000	66,000	70,000	10,000	N/A	10,000	80,000
FY 2022	7,000	81,000	88,000	10,000	N/A	10,000	98,000

2. Project Scope and Justification

Scope
The preliminary scope of the CRMF project is to construct a building to support the repair, maintenance, and testing of superconducting radiofrequency (SRF) accelerator components. These components include but are not limited to SRF cavities and cryomodules, high brightness electron injectors, and superconducting undulators. The building will need a concrete shielded enclosure for cryomodule testing, a control room, vertical test stand area for testing SRF cavities and components, a cryogenic refrigerator and distribution box, cryomodules handling fixtures used to insert and remove the cold mass from the cryomodule vacuum vessel, a cleanroom partitioned into class 10 and class 1000 areas, a loading and cryomodule preparation area, storage areas, and a 15 ton bridge crane for moving equipment from one area to another within the building.

Optional scope to be considered for inclusion in the project includes a dedicated SRF electron injector development and test area, which requires extending the envisioned building length by 30 feet, a 40 mega-electronvolt (MeV) SRF linac to provide the equipment and diagnostics necessary for an integrated injector test stand, and equipment to refurbish and test the niobium SRF cavities.

Justification
SC, through the two current BES construction projects, LCLS-II and LCLS-II-HE, is making over a $1,800,000,000 capital investment in an SRF linac at SLAC to support the science mission of DOE. The LCLS-II project is providing a 4 GeV SRF-based linear accelerator capable of providing 1 megahertz (MHz) electron pulses to create a free electron, x-ray laser. This machine contains 35 SRF cryomodules to accelerate the electrons to 4 GeV. The LCLS-II-HE will increase the energy of the LCLS-II linac to 8 GeV by providing an additional 20-22 SRF cryomodules of a similar design to the LCLS-II ones but operating at a higher accelerating gradient. SLAC has partnered with Fermi National Accelerator Laboratory (FNAL) and the Thomas Jefferson National Accelerator Facility (TJNAF) to provide the accelerating cryomodules. FNAL and TJNAF produce the cryomodules making use of specialized fabrication, assembly, and test capabilities available there. To make any repairs, the facilities must currently send the cryomodules back to either FNAL or TJNAF at an increased risk of damage, cost, and schedule delays.

The initial assumption was that cryomodules could be shipped back to the partner laboratories as needed for maintenance at a rate of 1 to 2 cryomodules per year. However, during construction of the LCLS-II facility it was determined that cryomodules could be damaged during transportation; transportation of cryomodules for repairs during operations would pose a risk to reliable facility operations. This approach also assumed that either FNAL or TJNAF would have the maintenance capabilities available when needed. At this time, the two partner laboratories have informed SLAC that they will need 6 to 12 months of advance notice to schedule maintenance or repairs to the SLAC hardware.

The proposed CRMF is designed to meet these challenges and will provide the capability to repair, maintain, and test SRF accelerator components, the primary one being the SRF cryomodules that make up the new superconducting accelerator being constructed by the LCLS-II and LCLS-II-HE construction projects. The facility will provide for the full disassembly and repair of the SRF cryomodule; the ability to disassemble, clean, and reassemble the SRF cavities and cavity string; testing capabilities for the full cryomodule; and separate testing capabilities for individual SRF cavities.

The photon energy range for LCLS-II-HE could be extended by lowering the emittance of the electron injector, which requires an R&D effort. The lack of an appropriate research and development (R&D) facility with testing capabilities has hindered progress in this area at SLAC. The CRMF project will provide this needed support to SLAC when constructed.

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

Key Performance Parameters (KPPs)
The KPPs are preliminary and may change as the project continues towards CD-2. At CD-2 approval, the KPPs will be baselined. The Threshold KPPs represent the minimum acceptable performance that the project must achieve. The Objective KPPs represent the desired project performance. Achievement of the Threshold KPPs will be a prerequisite for approval of CD-4, Project Completion.

Performance Measure	Threshold	Objective
Conventional Facilities Building Area	22,000 gross square feet	25,000 gross square feet
Electron Beam Energy	50 MeV	128 MeV
Cryogenic Cooling Capacity at 2K	100 Watts	250 Watts

3. Financial Schedule

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Estimated Cost (TEC)			
Design (TEC)			
FY 2021	1,000	1,000	–
FY 2022	1,000	1,000	1,650
Outyears	5,000	5,000	5,350
Total, Design (TEC)	**7,000**	**7,000**	**7,000**
Construction (TEC)			
Outyears	81,000	81,000	81,000
Total, Construction (TEC)	**81,000**	**81,000**	**81,000**
Total Estimated Cost (TEC)			
FY 2021	1,000	1,000	–
FY 2022	1,000	1,000	1,650
Outyears	86,000	86,000	86,350
Total, TEC	**88,000**	**88,000**	**88,000**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Other Project Cost (OPC)			
FY 2021	1,000	1,000	880
FY 2022	2,000	2,000	1,870
Outyears	7,000	7,000	7,250
Total, OPC	**10,000**	**10,000**	**10,000**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Project Cost (TPC)			
FY 2021	2,000	2,000	880
FY 2022	3,000	3,000	3,520
Outyears	93,000	93,000	93,600
Total, TPC	**98,000**	**98,000**	**98,000**

4. Details of Project Cost Estimate

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design	5,650	3,500	**N/A**
Design - Contingency	1,350	500	**N/A**
Total, Design (TEC)	**7,000**	**4,000**	**N/A**
Site Preparation	8,000	1,000	**N/A**
Equipment	7,400	35,000	**N/A**
Other Construction	46,850	15,500	**N/A**
Construction - Contingency	18,750	14,500	**N/A**
Total, Construction (TEC)	**81,000**	**66,000**	**N/A**
Total, TEC	**88,000**	**70,000**	**N/A**
Contingency, TEC	*20,100*	*15,000*	***N/A***
Other Project Cost (OPC)			
R&D	N/A	1,000	**N/A**
Conceptual Planning	500	1,000	**N/A**
Conceptual Design	5,500	2,000	**N/A**
Start-up	1,500	3,000	**N/A**
OPC - Contingency	2,500	3,000	**N/A**
Total, Except D&D (OPC)	**10,000**	**10,000**	**N/A**
Total, OPC	**10,000**	**10,000**	**N/A**
Contingency, OPC	*2,500*	*3,000*	***N/A***
Total, TPC	**98,000**	**80,000**	**N/A**
Total, Contingency (TEC+OPC)	***22,600***	***18,000***	***N/A***

5. Schedule of Appropriations Requests

(dollars in thousands)

Request Year	Type	Prior Years	FY 2021	FY 2022	Outyears	Total
FY 2021	TEC	—	1,000	—	69,000	70,000
	OPC	—	1,000	—	9,000	10,000
	TPC	—	2,000	—	78,000	80,000
FY 2022	TEC	—	1,000	1,000	86,000	88,000
	OPC	—	1,000	2,000	7,000	10,000
	TPC	—	2,000	3,000	93,000	98,000

6. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy	FY 2028
Expected Useful Life	25 years
Expected Future Start of D&D of this capital asset	FY 2053

Related Funding Requirements
(dollars in thousands)

	Annual Costs		Life Cycle Costs	
	Previous Total Estimate	Current Total Estimate	Previous Total Estimate	Current Total Estimate
Operations, Maintenance and Repair	N/A	5,500	N/A	286,000

Additional operations and maintenance costs are expected above the estimated costs to operate the LCLS-II facility. The estimate will be updated and additional details will be provided after CD-1, Approve Alternate Selection and Cost Range.

7. D&D Information

At this stage of project planning and development, SC anticipates that a new 22,000 to 25,000 gsf building may be constructed as part of this project.

8. Acquisition Approach

The CRMF Project will be sited at the SLAC National Accelerator Laboratory and will be acquired under the existing DOE Management and Operations contract for that laboratory.

SLAC will prepare a Conceptual Design Report for the CRMF project and demonstrate that they have the required project management systems in place to execute the project.

SLAC may choose to partner with other 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 similar facilities at other national laboratories, to the extent practicable. The project will fully exploit recent cost data from similar operating facilities in planning and budgeting. SLAC or partner laboratory staff may assist with completing the design of the technical systems. The selected contractor and/or subcontracted vendors with the necessary capabilities will fabricate technical equipment. All subcontracts will be competitively bid and awarded based on best value to the government.

Lessons learned from other SC projects and other similar facilities will be exploited fully in planning and executing CRMF.

19-SC-14, Second Target Station (STS), ORNL
Oak Ridge National Laboratory, Oak Ridge, Tennessee
Project is for Design and Construction

1. Summary, Significant Changes, and Schedule and Cost History

Summary

The FY 2022 Request for Second Target Station (STS) project is $32,000,000 of Total Estimated Cost (TEC) funding. This project has a preliminary Total Project Cost (TPC) range of $1,800,000,000 to $3,000,000,000. This cost range encompasses the most feasible preliminary alternatives. The preliminary TPC estimate is $2,242,000,000.

Significant Changes

STS was initiated in FY 2019. The most recent DOE Order 413.3B approved Critical Decision (CD) is CD-1, Approve Alternative Selection and Cost Range, approved on November 23, 2020. This Construction Project Data Sheet (CPDS) is an update of the FY 2021 CPDS and does not include a new start for FY 2022. Compared to the CD-0 estimates in FY 2009, there was a significant increase in the estimated TPC at CD-1. The increase is the result in escalation (CD-0 assumed CD-1 in FY 2013, CD-1 was actually granted in FY 2021), evolution in scope due to a deeper understanding of requirements and systems as a result of conceptual design, including project management and site preparation, and increased contingency (25 percent of CD-0 estimate vs. 39 percent of current estimate) due to understanding of pandemic impacts and better estimates of project risks.

In FY 2020, the project advanced the planning, research and development (R&D), and conceptual design and conducted technical design reviews for the major systems (target, instruments, controls, accelerator, and conventional facilities). In FY 2021, the project received CD-1 and continued planning, R&D, design, engineering, and other activities required to advance the STS project toward CD-2. The focus will be on maturing the accelerator, target, instrument, controls, and conventional civil construction subsystems. A commercial Architect/Engineer (AE) firm will be contracted to assist in advancing the planning, engineering, and design. Proposals from scientific community teams for world-class instrument concepts will be reviewed and eight will be included in the project. In FY 2022, the project will continue the FY 2021 activities of planning, R&D, and engineering to assist in maturing the project design, scope, cost, schedule and key performance parameters with continued emphasis on advancing the accelerator, target, instrument, controls, and conventional civil construction subsystems. A commercial Construction Manager/General Contractor firm will be contracted to work with the AE firm to assist in maturing the planning, engineering, and design with emphasis on the conventional civil construction plans and site preparation.

A Federal Project Director, certified to level III, has been assigned to this project and has approved this CPDS.

Critical Milestone History

Fiscal Year	CD-0	Conceptual Design Complete	CD-1	CD-2	Final Design Complete	CD-3	D&D Complete	CD-4
FY 2020	1/7/09	2Q FY 2022	2Q FY 2022	2Q FY 2023	2Q FY 2025	2Q FY 2024	N/A	4Q FY 2031
FY 2021	1/7/09	2Q FY 2021	2Q FY 2021	3Q FY 2024	3Q FY 2026	3Q FY 2025	N/A	2Q FY 2032
FY 2022	1/7/09	4/30/21	11/23/20	2Q FY 2025	4Q FY 2029	2Q FY 2025	N/A	2Q FY 2037

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 Alternative Selection and Cost Range
CD-2 – Approve 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

Project Cost History

(dollars in thousands)

Fiscal Year	TEC, Design	TEC, Construction	TEC, Total	OPC, Except D&D	OPC, D&D	OPC, Total	TPC
FY 2020	65,500	1,138,500	1,204,000	45,300	N/A	45,300	1,249,300
FY 2021	65,500	1,158,200	1,223,700	45,300	N/A	45,300	1,269,000
FY 2022[a]	333,000	1,810,000	2,143,000	99,000	N/A	99,000	2,242,000

2. Project Scope and Justification

Scope

To address the gap in advanced neutron sources and instrumentation, the STS project will design, build, install, and test the equipment necessary to provide the four primary elements of the new Spallation Neutron Source (SNS) facility: the neutron target and moderators; the accelerator systems; the instruments; and the conventional facilities. Costs for acceptance testing, integrated testing, and initial commissioning to demonstrate achievement of the Key Performance Parameters (KPPs) are included in the STS scope. The STS will be located in unoccupied space east of the existing First Target Station (FTS). The project requires approximately 350,000 ft^2 of new buildings, making conventional facility construction a major contributor to project costs.

Justification

The Basic Energy Sciences (BES) mission 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.” BES accomplishes its mission in part by operation of large-scale user facilities consisting of a complementary set of intense x-rays sources, neutron scattering centers, electron beam characterization capabilities, and research centers for nanoscale science.

In the area of neutron science, the scientific community conducted numerous studies since the 1970’s that have established the scientific justification and need for a very high-intensity pulsed neutron source in the U.S. Since 2007, when it began its user program at Oak Ridge National Laboratory (ORNL), the SNS has been fulfilling this need. In accordance with the 1996 Basic Energy Sciences Advisory Committee (BESAC) (Russell Panel) Report recommendation, SNS has many technical margins built into its systems to facilitate a power upgrade into the 2-4 megawatt (MW) range to maintain its position of scientific leadership in the future.

An upgraded SNS would enable many advances in the opportunities described in the 2015 BESAC report “Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science.” ORNL held four workshops to assess the neutron scattering needs in quantum condensed matter, soft matter, biology, and the frontiers in materials discovery. These four areas encompass and directly map to the transformative opportunities identified in the BES Grand Challenges update. Quantum materials map most directly to harnessing coherence in light and matter, while soft matter and biology

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

are aligned primarily with mastering hierarchical architectures and beyond-equilibrium matter, and frontiers in materials discovery explored many of the topics in beyond ideal materials and systems: understanding the critical roles of heterogeneity, interfaces, and disorder. As an example, while neutrons already play an important role in the areas of biology and soft matter, step change improvements in capability will be required to make full use of the unique properties of neutrons to meet challenges in mastering hierarchical architectures and beyond-equilibrium matter and understanding the critical roles of heterogeneity and interfaces. The uniform conclusion from all workshops was that in the areas of science covered, neutrons play a unique and pivotal role in understanding structure and dynamics in materials required to develop future technologies.

The STS will feature a proton beam that is highly concentrated to produce a very high density beam of protons that strikes a rotating solid tungsten target. The produced neutron beam illuminates moderators located above and below the target that will feed up to 22 experimental beamlines (eight within the STS project scope) with neutron beams conditioned for specific instruments. The small-volume cold neutron moderator system is geometrically optimized to deliver higher peak brightness neutrons.

The SNS Proton Power Upgrade (PPU) project, requested separately, will double the power of the SNS accelerator complex to 2.8 MW so that STS can use one out of every four proton pulses to produce cold neutron beams with the highest peak brightness of any current or projected neutron sources. The high-brightness pulsed source optimized for cold neutron production will operate at 15 Hz (as compared to FTS, which currently operates at 60 Hz, but will operate at 45 pulses/second when STS is operating) to provide the large time-of-flight intervals corresponding to the broad time and length scales required to characterize complex materials. The project will provide a series of kicker magnets to divert every fourth proton pulse away from the FTS to a new line feeding the STS. Additional magnets will further deflect the beam into the transport line to the new target. A final set of quadrupole magnets will tailor the proton beam shape and distribution to match the compact source design.

An initial set of eight best-in-class instruments, developed with input from the user community, are largely built on known and demonstrated technologies but will need some research and development to deliver unprecedented levels of performance. Advanced neutron optics designs are needed for high alignment and stability requirements. The lower repetition rate of STS pushes the chopper design to larger diameter rotating elements with tighter limits on allowed mechanical vibration. The higher peak neutron production of STS will put a greater demand on neutron detector technology.

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

Key Performance Parameters (KPPs)

The KPPs are preliminary and may change as the project continues towards CD-2. At CD-2 approval, the KPPs will be baselined. The Threshold KPPs represent the minimum acceptable performance that the project must achieve. The Objective KPPs represent the desired project performance. Achievement of the Threshold KPPs will be a prerequisite for approval of CD-4, Project Completion.

Performance Measure	Threshold	Objective
Demonstrate independent control of the proton beam on the two target stations	Operate beam to FTS at 45 pulses/s, with no beam to STS. Operate beam to STS at 15 Hz, with no beam to FTS. Operate with beam to both target stations 45 pulses/s at FTS and 15 Hz at STS.	Operate beam to FTS at 45 pulses/s, with no beam to STS. Operate beam to STS at 15 Hz, with no beam to FTS. Operate with beam to both target stations 45 pulses/s at FTS and 15 Hz at STS.
Demonstrate proton beam power on STS at 15 Hz	100 kW beam power	700 kW beam power
Measure STS neutron brightness	peak brightness of 2×10^{13} n/cm^2/sr/Å/s at 5 Å	peak brightness of 2×10^{14} n/cm^2/sr/Å/s at 5 Å
Beamlines transitioned to operations	8 beamlines successfully passed the integrated functional testing per the transition to operations parameters acceptance criteria	≥ 8 beamlines successfully passed the integrated functional testing per the transition to operations parameters acceptance criteria

3. Financial Schedule

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Estimated Cost (TEC)			
Design (TEC)			
FY 2019	1,000	1,000	–
FY 2020	20,000	20,000	–
FY 2021	29,000	29,000	37,000
FY 2022	32,000	32,000	37,500
Outyears	251,000	251,000	258,500
Total, Design (TEC)	**333,000**	**333,000**	**333,000**
Construction (TEC)			
Outyears	1,810,000	1,810,000	1,810,000
Total, Construction (TEC)	**1,810,000**	**1,810,000**	**1,810,000**
Total Estimated Cost (TEC)			
FY 2019	1,000	1,000	–
FY 2020	20,000	20,000	–
FY 2021	29,000	29,000	37,000
FY 2022	32,000	32,000	37,500
Outyears	2,061,000	2,061,000	2,068,500
Total, TEC	**2,143,000**	**2,143,000**	**2,143,000**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Other Project Cost (OPC)			
FY 2016	5,941	5,941	3,069
FY 2017	62	62	2,818
FY 2018	4,802	4,802	250
FY 2019	5,000	5,000	6,262
FY 2020	17,000	17,000	10,917
FY 2021	13,000	13,000	19,750
FY 2022	–	–	2,739
Outyears	53,195	53,195	53,195
Total, OPC	**99,000**	**99,000**	**99,000**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Project Cost (TPC)			
FY 2016	5,941	5,941	3,069
FY 2017	62	62	2,818
FY 2018	4,802	4,802	250
FY 2019	6,000	6,000	6,262
FY 2020	37,000	37,000	10,917
FY 2021	42,000	42,000	56,750
FY 2022	32,000	32,000	40,239
Outyears	2,114,195	2,114,195	2,121,695
Total, TPC	**2,242,000**	**2,242,000**	**2,242,000**

4. Details of Project Cost Estimate

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design	256,500	48,500	**N/A**
Design - Contingency	76,500	17,000	**N/A**
Total, Design (TEC)	**333,000**	**65,500**	**N/A**
Construction	1,291,500	864,700	**N/A**
Construction - Contingency	518,500	293,500	**N/A**
Total, Construction (TEC)	**1,810,000**	**1,158,200**	**N/A**
Total, TEC	**2,143,000**	**1,223,700**	**N/A**
Contingency, TEC	*595,000*	*310,500*	***N/A***
Other Project Cost (OPC)			
R&D	22,875	4,502	**N/A**
Conceptual Design	24,750	20,852	**N/A**
Start-up	20,250	8,621	**N/A**
OPC - Contingency	31,125	11,325	**N/A**
Total, Except D&D (OPC)	**99,000**	**45,300**	**N/A**
Total, OPC	**99,000**	**45,300**	**N/A**
Contingency, OPC	*31,125*	*11,325*	***N/A***
Total, TPC	**2,242,000**	**1,269,000**	**N/A**
Total, Contingency (TEC+OPC)	***626,125***	***321,825***	***N/A***

5. Schedule of Appropriations Requests

(dollars in thousands)

Request Year	Type	Prior Years	FY 2020	FY 2021	FY 2022	Outyears	Total
FY 2020	TEC	1,000	1,000	1,000	—	1,201,000	1,204,000
	OPC	11,500	—	1,000	—	32,800	45,300
	TPC	12,500	1,000	2,000	—	1,233,800	1,249,300
FY 2021	TEC	1,000	20,000	1,000	—	1,201,700	1,223,700
	OPC	15,805	17,000	1,000	—	11,495	45,300
	TPC	16,805	37,000	2,000	—	1,213,195	1,269,000
FY 2022	TEC	1,000	20,000	29,000	32,000	2,061,000	2,143,000
	OPC	15,805	17,000	13,000	—	53,195	99,000
	TPC	16,805	37,000	42,000	32,000	2,114,195	2,242,000

6. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy	FY 2037
Expected Useful Life	25 years
Expected Future Start of D&D of this capital asset	FY 2062

Related Funding Requirements
(dollars in thousands)

	Annual Costs		Life Cycle Costs	
	Previous Total Estimate	Current Total Estimate	Previous Total Estimate	Current Total Estimate
Operations, Maintenance and Repair	N/A	59,000	N/A	1,475,000

The numbers presented are the incremental operations and maintenance costs above the existing SNS facility without escalation. The estimate will be updated and additional details will be provided after CD-2, Approve Performance Baseline.

7. 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 ORNL	~350,000
Area of D&D in this project at ORNL	—
Area at ORNL to be transferred, sold, and/or D&D outside the project, including area previously "banked"	~350,000
Area of D&D in this project at other sites	—
Area at other sites to be transferred, sold, and/or D&D outside the project, including area previously "banked"	—
Total area eliminated	—

8. Acquisition Approach

DOE has determined that ORNL will acquire the STS project under the existing DOE Management and Operations (M&O) contract.

The M&O contractor prepared a Conceptual Design Report for the STS project and identified key design activities, requirements, and high-risk subsystem components 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 an ORNL-wide resource.

ORNL will design and procure the key technical subsystem components. Some technical system designs will require research and development activities. Preliminary cost estimates for most of these systems are based on operating experience of SNS and vendor estimates, while some first-of-a-kind systems are based on expert judgement. Vendors and/or partner labs with the necessary capabilities will fabricate the technical equipment. ORNL will competitively bid and award all subcontracts based on best value to the government. The M&O contractor's performance will be evaluated through the annual laboratory performance appraisal process.

Lessons learned from other Office of Science projects and other similar facilities will be exploited fully in planning and executing STS.

18-SC-10, Advanced Photon Source Upgrade (APS-U), ANL
Argonne National Laboratory
Project is for Design and Construction

1. Summary, Significant Changes, and Schedule and Cost History

Summary

The FY 2022 Request for the Advanced Photon Source-Upgrade (APS-U) project is $106,000,000. The project has a Total Project Cost (TPC) of $815,000,000.

Significant Changes

The APS-U became a line item project in FY 2018. The most recent approved DOE Order 413.3B critical decision is CD-3 (Approve Start of Construction), which was approved on July 25, 2019. CD-4, Approve Project Completion is projected for mid-FY 2026. There are no significant changes.

In FY 2020, APS-U completed the majority of equipment prototyping and development work and awarded most of the contracts for accelerator magnets, support structures, power supplies, vacuum chambers, experimental systems, front ends, and insertion devices needed to maintain the project schedule. Off-site space for storage was leased. Deliveries of the production first articles arrived for inspection and successfully passed acceptance testing. FY 2021 funding enables the advancement of the storage ring and experimental facilities final design, engineering, prototyping, testing, fabrication, procurement of baseline and spare hardware, integration, and installation, and enables site preparation and civil construction activities for the long beamline building. The project will continue receiving and inspecting hardware for the storage ring and experimental facilities and advance the integrated magnet module assembly. The FY 2022 Request will support continuing FY 2021 activities to advance the design, engineering, prototyping, testing, fabrication, procurement of baseline and spare hardware, integration, and installation for the storage ring and experimental facilities. Further civil construction associated with the long beamline building will occur. Completing final designs, system integration, testing, and assembly in preparation for the storage ring removal and installation during the experimental dark time, tentatively scheduled to begin in late June 2022, will be a high priority. COVID-19 may delay progress.

A Federal Project Director, certified to Level IV, has been assigned to this project and has approved this CPDS.

Critical Milestone History

Fiscal Year	CD-0	Conceptual Design Complete	CD-1	CD-2	Final Design Complete	CD-3	D&D Complete	CD-4
FY 2018	4/22/10	9/18/15	2/4/16	1Q FY 2019	2Q FY 2020	4Q FY 2019	N/A	1Q FY 2026
FY 2019	4/22/10	9/18/15	2/4/16	2Q FY 2019	4Q FY 2021	1Q FY 2020	N/A	2Q FY 2026
FY 2020	4/22/10	9/18/15	2/4/16	12/9/18	1Q FY 2022	1Q FY 2020	N/A	2Q FY 2026
FY 2021	4/22/10	9/18/15	2/4/16	12/9/18	1Q FY 2022	7/25/19	N/A	2Q FY 2026
FY 2022	4/22/10	9/18/15	2/4/16	12/9/18	1Q FY 2022	7/25/19	N/A	2Q FY 2026

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 Alternative Selection and Cost Range
CD-2 – Approve 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

Fiscal Year	Performance Baseline Validation	CD-3A	CD-3B
FY 2018	1Q FY 2019	8/30/12	10/6/16
FY 2019	2Q FY 2019	8/30/12	10/6/16
FY 2020	12/9/18	8/30/12	10/6/16
FY 2021	12/9/18	8/30/12	10/6/16
FY 2022	12/9/18	8/30/12	10/6/16

CD-3A – Approve Long-Lead Procurements for the Resonant Inelastic X-ray Scattering (RIXS) beamline.
CD-3B – Approve Long-Lead Procurements for accelerator components and associated systems.

Project Cost History

(dollars in thousands)

Fiscal Year	TEC, Design	TEC, Construction	TEC, Total	OPC, Except D&D	OPC, D&D	OPC, Total	TPC
FY 2018	157,015	561,985	719,000	51,000	N/A	51,000	770,000
FY 2019	167,000	590,100	757,100	12,900	N/A	12,900	770,000
FY 2020	162,825	633,675	796,500	18,500	N/A	18,500	815,000
FY 2021	190,425	606,075	796,500	18,500	N/A	18,500	815,000
FY 2022	189,638	606,862	796,500	18,500	N/A	18,500	815,000

2. Project Scope and Justification

Scope

The APS-U project will upgrade the existing APS to provide scientists with an x-ray light source possessing world-leading transverse coherence and extreme brightness. The project's scope includes a new very low emittance multi-bend achromat (MBA) lattice storage ring in the existing tunnel, new permanent magnet and superconducting insertion devices optimized for brightness and flux, new or upgraded front-ends, and any required modifications to the linac, booster, and radiofrequency systems. The project will also construct new beamlines and incorporate substantial refurbishment of existing beamlines, along with new optics and detectors that will enable the beamlines to take advantage of the improved accelerator performance. Two best-in-class beamlines require conventional civil construction to extend the beamlines beyond the existing APS Experimental Hall to achieve the desired nano-focused beam spot size.

Justification

The BES mission 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." APS-U will provide the nation's researchers with a world-class scientific user facility for mission-focused research and advanced scientific discovery.

Worldwide investments in accelerator-based x-ray light source user facilities threaten U.S. leadership in light source technology within the next 6 to 10 years. The European Synchrotron Radiation Facility (ESRF) in France, PETRA-III in Germany, and SPring-8 in Japan are well into campaigns of major upgrades of beamlines and are also incorporating technological advancements in accelerator science to enhance performance for hard x-ray energies (>20 keV). In 2019, China initiated construction of the High Energy Photon Source (HEPS), a next-generation six giga-electronvolt (GeV) hard x-ray synchrotron light source. The ESRF upgrade, ESRF-EBS, was completed in early 2020.

The APS upgrade will provide a world-class hard x-ray synchrotron radiation facility, with 100 to 1000 times increased brightness and coherent flux over the current APS, and will be a unique asset in the U.S. portfolio of scientific user facilities. The APS-U is a critical and cost-effective next step in the photon science strategy that will keep the U.S. at the forefront of scientific research, combining with other facilities to give the U.S. a complementary set of storage ring and free-electron laser x-ray light sources.

The high-brightness, high-energy penetrating hard x-rays will provide a unique scientific capability directly relevant to probing real-world materials and applications in energy, the environment, new and improved materials, and biological studies. The APS upgrade will ensure that the APS remains a world leader in hard x-ray science.

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

Key Performance Parameters (KPPs)
The Threshold KPPs represent the minimum acceptable performance that the project must achieve. The Objective KPPs represent the desired project performance. Achievement of the Threshold KPPs is a prerequisite for approval of CD-4, Project Completion.

Performance Measure	Threshold	Objective
Storage Ring Energy	> 5.7 GeV, with systems installed for 6 GeV operation	6 GeV
Beam Current	≥ 25 milliamps (mA)in top-up injection mode with systems installed for 200 mA operation	200 mA in top-up injection mode
Horizontal Emittance	< 130 pm-rad at 25 mA	≤ 42 pm-rad at 200 mA
Brightness @ 20 keV[1]	> 1×10^{20}	1×10^{22}
Brightness @ 60 keV[1]	> 1×10^{19}	1×10^{21}
New APS-U Beamlines Transitioned to Operations	7	≥ 9

[1]Units = photons/sec/mm^2/mrad^2/0.1% BW

3. Financial Schedule

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Estimated Cost (TEC)			
Design (TEC)			
FY 2012	19,200	19,200	9,095
FY 2013	15,000	15,000	17,825
FY 2014	17,015	17,015	12,889
FY 2015	20,000	20,000	19,782
FY 2016	20,000	20,000	22,529
FY 2017	34,785	34,785	23,873
FY 2018	26,000	26,000	23,829
FY 2019	14,650	14,650	23,985
FY 2020	22,988	22,988	28,486
FY 2021	–	–	7,227
FY 2022	–	–	118
Total, Design (TEC)	**189,638**	**189,638**	**189,638**
Construction (TEC)			
FY 2012	800	800	–
FY 2013	5,000	5,000	3,391
FY 2014	2,985	2,985	4,534
FY 2015	–	–	573
FY 2017	7,715	7,715	389
FY 2018	67,000	67,000	6,307
FY 2019	113,150	113,150	24,425
FY 2020	147,012	147,012	55,859
FY 2021	160,000	160,000	229,709
FY 2022	101,000	101,000	232,058
Outyears	2,200	2,200	49,617
Total, Construction (TEC)	**606,862**	**606,862**	**606,862**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Estimated Cost (TEC)			
FY 2012	20,000	20,000	9,095
FY 2013	20,000	20,000	21,216
FY 2014	20,000	20,000	17,423
FY 2015	20,000	20,000	20,355
FY 2016	20,000	20,000	22,529
FY 2017	42,500	42,500	24,262
FY 2018	93,000	93,000	30,136
FY 2019	127,800	127,800	48,410
FY 2020	170,000	170,000	84,345
FY 2021	160,000	160,000	236,936
FY 2022	101,000	101,000	232,176
Outyears	2,200	2,200	49,617
Total, TEC	**796,500**	**796,500**	**796,500**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Other Project Cost (OPC)			
FY 2010	1,000	1,000	587
FY 2011	7,500	7,500	3,696
FY 2012	–	–	4,217
FY 2022	5,000	5,000	4,400
Outyears	5,000	5,000	5,600
Total, OPC	**18,500**	**18,500**	**18,500**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Project Cost (TPC)			
FY 2010	1,000	1,000	587
FY 2011	7,500	7,500	3,696
FY 2012	20,000	20,000	13,312
FY 2013	20,000	20,000	21,216
FY 2014	20,000	20,000	17,423
FY 2015	20,000	20,000	20,355
FY 2016	20,000	20,000	22,529
FY 2017	42,500	42,500	24,262
FY 2018	93,000	93,000	30,136
FY 2019	127,800	127,800	48,410
FY 2020	170,000	170,000	84,345
FY 2021	160,000	160,000	236,936
FY 2022	106,000	106,000	236,576
Outyears	7,200	7,200	55,217
Total, TPC	**815,000**	**815,000**	**815,000**

Note – In FY 2021, the Office of Science reprogrammed $2,200,000 of FY 2019 funds to the LCLS-II project at SLAC. The FY 2019 Budget Authority in the table above reflects this reprogramming and additional funds are required in the outyears to maintain the project profile.

4. **Details of Project Cost Estimate**

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design	187,921	182,825	166,962
Design - Contingency	1,717	7,600	9,696
Total, Design (TEC)	**189,638**	**190,425**	**176,658**
Equipment	478,809	461,675	465,180
Other Construction	17,000	17,000	17,000
Construction - Contingency	111,053	127,400	137,662
Total, Construction (TEC)	**606,862**	**606,075**	**619,842**
Total, TEC	**796,500**	**796,500**	**796,500**
Contingency, TEC	*112,770*	*135,000*	*147,358*
Other Project Cost (OPC)			
Conceptual Planning	1,000	1,000	1,000
Conceptual Design	7,500	7,500	7,500
Start-up	7,570	7,100	7,100
OPC - Contingency	2,430	2,900	2,900
Total, Except D&D (OPC)	**18,500**	**18,500**	**18,500**
Total, OPC	**18,500**	**18,500**	**18,500**
Contingency, OPC	*2,430*	*2,900*	*2,900*
Total, TPC	**815,000**	**815,000**	**815,000**
Total, Contingency (TEC+OPC)	***115,200***	***137,900***	***150,258***

5. Schedule of Appropriations Requests

(dollars in thousands)

Request Year	Type	Prior Years	FY 2020	FY 2021	FY 2022	Outyears	Total
FY 2018	TEC	244,272	152,419	160,000	—	162,309	719,000
	OPC	8,500	—	5,000	—	37,500	51,000
	TPC	252,772	152,419	165,000	—	199,809	770,000
FY 2019	TEC	222,500	150,000	159,780	—	224,820	757,100
	OPC	8,500	—	—	—	4,400	12,900
	TPC	231,000	150,000	159,780	—	229,220	770,000
FY 2020	TEC	365,500	150,000	160,000	—	121,000	796,500
	OPC	8,500	—	5,000	—	5,000	18,500
	TPC	374,000	150,000	165,000	—	126,000	815,000
FY 2021	TEC	365,500	170,000	150,000	—	111,000	796,500
	OPC	8,500	—	—	—	10,000	18,500
	TPC	374,000	170,000	150,000	—	121,000	815,000
FY 2022	TEC	363,300	170,000	160,000	101,000	2,200	796,500
	OPC	8,500	—		5,000	5,000	18,500
	TPC	371,800	170,000	160,000	106,000	7,200	815,000

Note – In FY 2021, the Office of Science reprogrammed $2,200,000 of FY 2019 funds to the LCLS-II project at SLAC. The FY 2022 Request in the table above reflects this reprogramming and additional funds are required in the outyears to maintain the project profile.

6. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy	FY 2026
Expected Useful Life	25 years
Expected Future Start of D&D of this capital asset	FY 2051

Related Funding Requirements
(dollars in thousands)

	Annual Costs		Life Cycle Costs	
	Previous Total Estimate	Current Total Estimate	Previous Total Estimate	Current Total Estimate
Operations, Maintenance and Repair	N/A	18,000	N/A	450,000

The numbers presented are the incremental operations and maintenance costs above the existing APS facility without escalation. The estimate will be updated will be updated as the project is executed.

7. 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 ANL	23,000-27,000
Area of D&D in this project at ANL	—
Area at ANL to be transferred, sold, and/or D&D outside the project, including area previously "banked"	23,000-27,000
Area of D&D in this project at ANL	—
Area at other sites to be transferred, sold, and/or D&D outside the project, including area previously "banked"	—
Total area eliminated	—

Approximately 23,000-27,000 square feet of new construction is anticipated for the long beamline building, which will house two APS-U beamlines extending beyond the current APS experimental facilities and the support laboratories.

8. Acquisition Approach

ANL will acquire the APS-U project under the existing DOE Management and Operations (M&O) contract between DOE and UChicago Argonne, LLC. The acquisition of equipment and systems for large research facilities is within the scope of the DOE contract for the management and operations of ANL and consistent with the general expectation of the responsibilities of DOE M&O contractors.

ANL will have prime responsibility for oversight of all contracts required to execute this project, which will include managing the design and construction of the APS-U accelerator incorporating an MBA magnet lattice, insertion devices, front ends, beamlines/experimental stations, and any required modifications to the linac, booster, and radiofrequency systems. ANL has established an APS-U project organization with project management, procurement management, and Environment, Safety and Health (ES&H) management with staff qualified to specify, select and oversee procurement and installation of the accelerator and beamline components and other technical equipment. ANL will procure these items through competitive bids based on a 'best value' basis from a variety of sources, depending on the item, and following all applicable ANL procurement requirements. The APS-U project will most likely be accomplished using the design-bid-fabricate method. This proven approach provides the project with direct control over the accelerator components and beamline design, equipment specification and selection, and all contractors. The M&O contractor's performance will be evaluated through the annual laboratory performance appraisal process.

18-SC-11, Spallation Neutron Source Proton Power Upgrade (PPU), ORNL
Oak Ridge National Laboratory, Oak Ridge, Tennessee
Project is for Design and Construction

1. Summary, Significant Changes, and Schedule and Cost History

Summary

The FY 2022 Request for the Proton Power Upgrade (PPU) project is $17,000,000 of Total Estimated Cost (TEC) funding. The Total Project Cost (TPC) is $271,600,000.

Significant Changes

PPU was initiated in FY 2018. The most recent DOE Order 413.3B approved Critical Decision (CD) is a combined CD-2, Approve Performance Baseline and CD-3, Approve Start of Construction, approved on October 6, 2020. CD-4, Approve Project Completion, is anticipated at the end of FY 2028.

In FY 2020, the project held successful CD-2/3 cost and project reviews for baseline and start of construction readiness and continued target development in coordination with Spallation Neutron Source (SNS) operations target management plans. All CD-3A long-lead procurement contracts have been placed and are ~75% complete. Additional long-lead procurement authority (CD-3B), approved in late FY 2019 and executed in FY 2020, will advance the klystron gallery buildout, radiofrequency (RF) and high voltage procurements, and cryomodule hardware procurements, delivery and assembly. In FY 2021, the project will continue R&D, engineering, prototyping, preliminary and final design, testing, fabrication, procurement of baseline and spare hardware, and component integration and installation and civil construction, focusing on initial target procurement, initial cryomodule production, and continued RF equipment procurement, and will initiate equipment installation in the klystron gallery. In FY 2022, the project will prioritize these continuing activities of R&D, engineering, prototyping, final design, testing, fabrication, procurement of baseline and spare hardware, component integration and installation, and civil construction site preparation, with priority on continuing RF equipment installation in the klystron gallery, cryomodule assembly, first complete cryomodule receipt, and advancing the target knowledge base by running the first PPU test target during SNS operations.

A Federal Project Director, certified to level II, has been assigned to this project and has approved this CPDS.

Critical Milestone History

Fiscal Year	CD-0	Conceptual Design Complete	CD-1	CD-2	Final Design Complete	CD-3	D&D Complete	CD-4
FY 2020	1/7/09	8/1/17	4/4/18	2Q FY 2021	4Q FY 2022	3Q FY 2022	N/A	3Q FY 2027
FY 2021	1/7/09	8/1/17	4/4/18	2Q FY 2021	4Q FY 2022	2Q FY 2021	N/A	3Q FY 2027
FY 2022	1/7/09	8/1/17	4/4/18	10/6/20	1Q FY 2023	10/6/20	N/A	4Q FY 2028

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 Alternative Selection and Cost Range
CD-2 – Approve 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

Fiscal Year	Performance Baseline Validation	CD-3A	CD-3B
FY 2020	2Q FY 2021	10/5/18	2Q FY 2020
FY 2021	2Q FY 2021	10/5/18	9/3/19
FY 2022	10/6/20	10/5/18	9/3/19

CD-3A – Approve Long-Lead Procurements, niobium material, cryomodule cavities, and related cryomodule procurements.
CD-3B – Approve Long-Lead Procurements, klystron gallery buildout, RF procurements, and cryomodule hardware.

Project Cost History

(dollars in thousands)

Fiscal Year	TEC, Design	TEC, Construction	TEC, Total	OPC, Except D&D	OPC, D&D	OPC, Total	TPC
FY 2020	27,300	210,000	237,300	12,700	N/A	12,700	250,000
FY 2021	46,700	189,502	236,202	13,798	N/A	13,798	250,000
FY 2022	40,000	217,802	257,802	13,798	N/A	13,798	271,600

2. Project Scope and Justification

Scope

The PPU project will design, build, install, and test the equipment necessary to double the accelerator power from 1.4 megawatts (MW) to 2.8 MW, upgrade the existing SNS target system to accommodate beam power up to 2 MW, and deliver a 2 MW qualified target. PPU includes the provision for a stub-out in the SNS transport line to the existing target to facilitate rapid connection to a new proton beamline. The project also includes modifications to some buildings and services.

Justification

The Basic Energy Sciences (BES) mission 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." BES accomplishes its mission in part by operating large-scale user facilities consisting of a complementary set of intense x-ray sources, neutron scattering centers, electron beam characterization capabilities, and research centers for nanoscale science.

In the area of neutron science, numerous studies by the scientific community since the 1970s have established the scientific justification and need for a very high-intensity pulsed neutron source in the U.S. The SNS, which began its user program at Oak Ridge National Laboratory (ORNL) in 2007, currently fulfills the need. The SNS was designed to be upgradeable so as to maintain its position of scientific leadership in the future, in accordance with the 1996 Basic Energy Sciences Advisory Committee (BESAC) (Russell Panel) Report recommendation, and many technical margins were built into the SNS systems to facilitate a power upgrade into the 2 - 4 MW range with the ability to extract some of that power to a second target station.

An upgraded SNS will enable many advances in the opportunities described in the 2015 BESAC report "Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science." Four workshops were held by ORNL to assess the neutron scattering needs in quantum condensed matter, soft matter, biology, and the frontiers in materials discovery. These four areas encompass and directly map to the transformative opportunities identified in the BES Grand Challenges update. Quantum materials map most directly to harnessing coherence in light and matter, while soft matter and biology align primarily with mastering hierarchical architectures and beyond-equilibrium matter, and frontiers in materials discovery explored many of the topics in beyond ideal materials and systems: understanding the critical roles of heterogeneity, interfaces, and disorder. As an example, while neutrons already play an important role in the areas of biology and soft matter, step change improvements in capability will be required to make full use of the unique properties of neutrons to meet challenges in mastering hierarchical architectures and beyond-equilibrium matter and understanding the critical roles of heterogeneity and interfaces. The uniform conclusion from all of the workshops was that, in the areas of science covered, neutrons play a unique and pivotal role in understanding structure and dynamics in materials required to develop future technologies.

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

Key Performance Parameters (KPPs)
The Threshold KPPs, 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.

Performance Measure	Threshold	Objective
Beam power on target	1.7 MW at 1.25 giga-electron volts (GeV)	2.0 MW at 1.3 GeV
Beam energy	1.25 GeV	1.3 GeV
Target reliability lifetime without target failure	1,250 hours at 1.7 MW	1,250 hours at 2.0 MW
Stored beam intensity in ring	$\geq 1.6 \times 10^{14}$ protons at 1.25 GeV	$\geq 2.24 \times 10^{14}$ protons at 1.3 GeV

3. Financial Schedule

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Estimated Cost (TEC)			
Design (TEC)			
FY 2018	5,000	5,000	2,655
FY 2019	16,000	16,000	13,109
FY 2020	14,700	14,700	12,510
FY 2021	3,300	3,300	7,360
FY 2022	1,000	1,000	3,480
Outyears	–	–	886
Total, Design (TEC)	**40,000**	**40,000**	**40,000**
Construction (TEC)			
FY 2018	31,000	31,000	1,794
FY 2019	44,000	44,000	8,018
FY 2020	45,300	45,300	28,564
FY 2021	48,700	48,700	68,670
FY 2022	16,000	16,000	64,950
Outyears	32,802	32,802	45,806
Total, Construction (TEC)	**217,802**	**217,802**	**217,802**
Total Estimated Cost (TEC)			
FY 2018	36,000	36,000	4,449
FY 2019	60,000	60,000	21,127
FY 2020	60,000	60,000	41,074
FY 2021	52,000	52,000	76,030
FY 2022	17,000	17,000	68,430
Outyears	32,802	32,802	46,692
Total, TEC	**257,802**	**257,802**	**257,802**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Other Project Cost (OPC)			
FY 2016	4,059	4,059	1,267
FY 2017	6,739	6,739	3,773
FY 2018	–	–	3,004
FY 2019	–	–	1,567
FY 2020	–	–	124
FY 2021	3,000	3,000	517
FY 2022	–	–	489
Outyears	–	–	3,057
Total, OPC	**13,798**	**13,798**	**13,798**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Project Cost (TPC)			
FY 2016	4,059	4,059	1,267
FY 2017	6,739	6,739	3,773
FY 2018	36,000	36,000	7,453
FY 2019	60,000	60,000	22,694
FY 2020	60,000	60,000	41,198
FY 2021	55,000	55,000	76,547
FY 2022	17,000	17,000	68,919
Outyears	32,802	32,802	49,749
Total, TPC	**271,600**	**271,600**	**271,600**

4. Details of Project Cost Estimate

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design	32,000	38,800	32,000
Design - Contingency	8,000	7,900	8,000
Total, Design (TEC)	**40,000**	**46,700**	**40,000**
Construction	163,452	137,702	163,452
Construction - Contingency	54,350	51,800	54,350
Total, Construction (TEC)	**217,802**	**189,502**	**217,802**
Total, TEC	**257,802**	**236,202**	**257,802**
Contingency, TEC	*62,350*	*59,700*	*62,350*
Other Project Cost (OPC)			
R&D	2,408	2,800	2,408
Conceptual Design	7,250	6,498	7,250
Other OPC Costs	3,480	1,300	3,480
OPC - Contingency	660	3,200	660
Total, Except D&D (OPC)	**13,798**	**13,798**	**13,798**
Total, OPC	**13,798**	**13,798**	**13,798**
Contingency, OPC	*660*	*3,200*	*660*
Total, TPC	**271,600**	**250,000**	**271,600**
Total, Contingency (TEC+OPC)	***63,010***	***62,900***	***63,010***

5. Schedule of Appropriations Requests

(dollars in thousands)

Request Year	Type	Prior Years	FY 2020	FY 2021	FY 2022	Outyears	Total
FY 2020	TEC	96,000	5,000	30,000	—	106,300	237,300
	OPC	10,300	—	—	—	2,400	12,700
	TPC	106,300	5,000	30,000	—	108,700	250,000
FY 2021	TEC	96,000	60,000	5,000	—	75,202	236,202
	OPC	10,798	—	3,000	—	—	13,798
	TPC	106,798	60,000	8,000	—	75,202	250,000
FY 2022	TEC	96,000	60,000	52,000	17,000	32,802	257,802
	OPC	10,798	—	3,000	—		13,798
	TPC	106,798	60,000	55,000	17,000	32,802	271,600

6. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy	FY 2028
Expected Useful Life	40 years
Expected Future Start of D&D of this capital asset	FY 2068

Related Funding Requirements
(dollars in thousands)

	Annual Costs		Life Cycle Costs	
	Previous Total Estimate	**Current Total Estimate**	**Previous Total Estimate**	**Current Total Estimate**
Operations, Maintenance and Repair	N/A	9,325	N/A	373,000

7. 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 ORNL	3,000-4,000
Area of D&D in this project at ORNL	—
Area at ORNL to be transferred, sold, and/or D&D outside the project, including area previously "banked"	3,000-4,000
Area of D&D in this project at other sites	—
Area at other sites to be transferred, sold, and/or D&D outside the project, including area previously "banked"	—
Total area eliminated	—

8. Acquisition Approach

DOE has determined that the PPU project will be acquired by ORNL under the existing DOE Management and Operations (M&O) contract.

The M&O contractor has completed a Conceptual Design Report for the PPU project and identified key design activities, requirements, and high-risk subsystem components 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 an ORNL-wide resource.

ORNL will partner with other laboratories for design and procurement of key technical subsystem components. Some technical system designs will require research and development activities. Cost estimates for these systems are based on operating experience of SNS and vendor quotes. ORNL, partner laboratory staff, and/or vendors will complete the design of the technical systems. Vendors and/or partner labs with the necessary capabilities will fabricate technical equipment. All subcontracts will be competitively bid and awarded based on best value to the government.

Lessons learned from other Office of Science projects and other similar facilities will be exploited fully in planning and executing PPU. The M&O contractor's performance will be evaluated through the annual laboratory performance appraisal process.

18-SC-12, Advanced Light Source Upgrade (ALS-U), LBNL
Lawrence Berkeley National Laboratory
Project is for Design and Construction

1. Summary, Significant Changes, and Schedule and Cost History

Summary

The FY 2022 Request for the Advanced Light Source Upgrade (ALS-U) project is $75,100,000 of Total Estimated Cost (TEC) funding. The most recent DOE Order 413.3B approved Critical Decision (CD) is CD-2, Approve Performance Baseline, approved on April 2, 2021. The project has a Total Project Cost (TPC) of $590,000,000.

Significant Changes

The ALS-U was initiated in FY 2019. In FY 2020, the project initiated long lead procurements as approved at CD-3A, and continued with planning, engineering, design, research and development (R&D), and prototyping activities. FY 2021 funding continues the support of planning, engineering, design, R&D, prototyping activities, and long-lead procurements. FY 2022 funding will continue support of planning, engineering, design, R&D, prototyping, and procurements of both long-lead and normal construction items.

The project took on additional scope which included adding radiation shielding and safety-mandated seismic structural upgrades to the ALS facility to protect the ALS-U investment. The additional scope, along with maturing designs, increased the project cost point estimate to $590,000,000.

A Federal Project Director, certified to Level III, has been assigned to this project and has approved this CPDS.

Critical Milestone History

Fiscal Year	CD-0	Conceptual Design Complete	CD-1	CD-2	Final Design Complete	CD-3	D&D Complete	CD-4
FY 2019	9/27/16	4Q FY 2019	4Q FY 2019	4Q FY 2020	4Q FY 2022	4Q FY 2021	N/A	4Q FY 2026
FY 2020	9/27/16	4/30/18	9/21/18	2Q FY 2021	4Q FY 2021	1Q FY 2022	N/A	2Q FY 2028
FY 2021	9/27/16	4/30/18	9/21/18	2Q FY 2021	4Q FY 2021	1Q FY 2022	N/A	2Q FY 2028
FY 2022	9/27/16	4/30/18	9/21/18	4/2/21	2Q FY 2022	3Q FY 2022	N/A	4Q FY 2029

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 Alternative Selection and Cost Range
CD-2 – Approve 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

Fiscal Year	Performance Baseline Validation	CD-3A
FY 2019	4Q FY 2020	4Q FY 2020
FY 2020	2Q FY 2021	4Q FY 2019
FY 2021	2Q FY 2021	12/19/19
FY 2022	4/2/21	12/19/19

CD-3A – Approve Long-Lead Procurements scope included the equipment required for the electron accumulator ring.

Project Cost History

(dollars in thousands)

Fiscal Year	TEC, Design	TEC, Construction	TEC, Total	OPC, Except D&D	OPC, D&D	OPC, Total	TPC
FY 2019	39,000	243,000	282,000	38,000	N/A	38,000	320,000
FY 2020	89,750	248,250	338,000	30,000	N/A	30,000	368,000
FY 2021	89,750	290,450	380,200	30,000	N/A	30,000	410,200
FY 2022	135,711	426,289	562,000	28,000	N/A	28,000	590,000

2. Project Scope and Justification

Scope

The ALS-U project will upgrade the existing ALS facility by replacing the existing electron storage ring with a new electron storage ring based on a multi-bend achromat (MBA) lattice design to provide a soft x-ray source that is orders of magnitude brighter—a 10-1000 times increase in brightness over the current ALS—and to provide a significantly higher fraction of coherent light in the soft x-ray region (approximately 50-2,000 electronvolts [eV]) than is currently available at ALS. The project will replace the existing triple-bend achromat storage ring with a new, high-performance storage ring based on a nine-bend achromat design. In addition, the project will add a low-emittance, full-energy accumulator ring to the existing tunnel inner shield wall to enable on- and off-axis, swap-out injection and extraction into and from the new storage ring using fast kicker magnets. The new source will require upgrading x-ray optics on existing beamlines with some beamlines being realigned or relocated. The project adds two new undulator beamlines that are optimized for the novel science made possible by the beam's new high coherent flux. The project intends to reuse the existing building, utilities, electron gun, linac, and booster synchrotron equipment currently at ALS. Prior to CD-2, the scope was increased to include radiation shielding and safety-mandated seismic structural upgrades to the ALS facility. With an aggressive accelerator design, ALS-U will provide the highest coherent flux of any existing or planned storage ring facility worldwide, up to a photon energy of about 3.5 keV. This range covers the entire soft x-ray regime.

Justification

At this time, our ability to observe and understand materials and material phenomena in real-time and as they emerge and evolve is limited. Soft x-rays (approximately 50 to 2,000 eV) are ideally suited for revealing the chemical, electronic, and magnetic properties of materials, as well as the chemical reactions that underpin these properties. This knowledge is crucial for the design and control of new advanced materials that address the challenges of new energy technologies.

Existing storage ring light sources lack a key attribute that would revolutionize x-ray science: stable, nearly continuous soft x-rays with high brightness and high coherent flux—that is, smooth, well organized soft x-ray wave fronts. Such a stable, high brightness, high coherent flux source would enable 3D imaging with nanometer resolution and the measurement of spontaneous nanoscale motion with nanosecond resolution—all with electronic structure sensitivity.

Currently, BES operates advanced ring-based light sources that produce soft x-rays. The NSLS-II, commissioned in 2015, is the brightest soft x-ray source in the U.S. The ALS, completed in 1993, is competitive with NSLS-II for x-rays below 200 eV but not above that. NSLS-II is somewhat lower in brightness than the new Swedish light source, MAX-IV, which began user operations in 2017 and represents the first use of a MBA lattice design in a light source facility. Neither NSLS-II nor ALS make use of the newer MBA lattice design. Switzerland's SLS-2 (an MBA-based design in the planning stage) will be a brighter soft x-ray light source than both NSLS-II and MAX-IV when it is built and brought into operation. These international light sources, and those that follow, will present a significant challenge to the U.S. light source community to provide competitive x-ray sources to domestic users. Neither NSLS-II nor ALS soft x-ray light sources possess sufficient brightness or coherent flux to provide the capability to meet the mission need in their current configurations.

BES is currently supporting two major light source upgrade projects, the APS-U and LCLS-II. These two projects will upgrade existing x-ray facilities in the U.S. and will provide significant increases in brightness and coherent flux. These upgrades will not address the specific research needs that demand stable, nearly continuous soft x-rays with high brightness and high coherence.

APS-U, which is under construction at ANL, will deploy the MBA lattice design optimized for its higher 6 GeV electron energy and to produce higher energy (hard) x-rays in the range of 10-100 keV. Because the ring will be optimized for high energy, the soft x-ray light it produces will not be sufficiently bright to meet the research needs described above.

LCLS-II, which is under construction at SLAC, is a high repetition rate (up to 1 MHz) free electron laser (FEL) designed to produce high brightness, coherent x-rays, but in extremely short bursts rather than as a nearly continuous beam. Storage rings offer higher stability than FELs. In addition, there is a need for a facility that can support a larger number of concurrent experiments than is possible with LCLS-II in its current configuration. This is critical for serving the large and expanding soft x-ray research community. LCLS-II will not meet this mission need.

The existing ALS is a 1.9 GeV storage ring operating at 500 milliamps (mA) of beam current. It is optimized to produce intense beams of soft x-rays, which offer spectroscopic contrast, nanometer-scale resolution, and broad temporal sensitivity. The ALS facility includes an accelerator complex and photon delivery system that are capable of providing the foundations for an upgrade that will achieve world-leading soft x-ray coherent flux. The existing ALS provides a ready-made foundation, including conventional facilities, a $500,000,000 scientific infrastructure investment and a vibrant user community of over 2,500 users per year already attuned to the potential scientific opportunities an upgrade offers. The facility also includes extensive (up to 40) simultaneously operating beamlines and instrumentation, an experimental hall, computing resources, ancillary laboratories, offices, and related infrastructure that will be heavily utilized in an upgrade scenario. Furthermore, the upgrade leverages the ALS staff, who are experts in the scientific and technical aspects of the proposed upgrade.

In summary, the capabilities at our existing x-ray light source facilities are insufficient to develop the next generation of tools that combine high resolution spatial imaging together with precise energy resolving spectroscopic techniques in the soft x-ray range. To enable these cutting edge experimental techniques, it is necessary to possess an ultra-bright source of soft x-ray light that generates the high coherent x-ray flux required to resolve nanometer-scale features and interactions, and to allow the real-time observation and understanding of materials and phenomena as they emerge and evolve. Developing such a light source will ensure the U.S. has the tools to maintain its leadership in soft x-ray science and will significantly accelerate the advancement of the fundamental sciences that underlie a broad range of emerging and future energy applications.

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

Key Performance Parameters (KPPs)

The Threshold KPPs represent the minimum acceptable performance that the project must achieve. The Objective KPPs represent the desired project performance. Achievement of the Threshold KPPs will be a prerequisite for approval of CD-4, Project Completion.

Performance Measure	Threshold	Objective
Storage Ring Energy	≥ 1.9 GeV	2.0 GeV
Beam Current	> 25 mA	500 mA
Horizontal Emittance	< 150 pm-rad	< 85 pm-rad
Brightness @ 1 keV[1]	$> 2 \times 10^{19}$	$\geq 2 \times 10^{21}$
New MBA Beamlines	2	≥ 2

[1]Units = photons/sec/0.1% BW/mm2/mrad2

3. Financial Schedule

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Estimated Cost (TEC)			
Design (TEC)			
FY 2018	16,000	16,000	–
FY 2019	35,000	35,000	22,054
FY 2020	10,000	10,000	33,101
FY 2021	40,000	40,000	39,146
FY 2022	34,711	34,711	35,000
Outyears	–	–	6,410
Total, Design (TEC)	**135,711**	**135,711**	**135,711**
Construction (TEC)			
FY 2019	25,000	25,000	–
FY 2020	50,000	50,000	3,520
FY 2021	22,000	22,000	35,000
FY 2022	40,389	40,389	40,000
Outyears	288,900	288,900	347,769
Total, Construction (TEC)	**426,289**	**426,289**	**426,289**
Total Estimated Cost (TEC)			
FY 2018	16,000	16,000	–
FY 2019	60,000	60,000	22,054
FY 2020	60,000	60,000	36,621
FY 2021	62,000	62,000	74,146
FY 2022	75,100	75,100	75,000
Outyears	288,900	288,900	354,179
Total, TEC	**562,000**	**562,000**	**562,000**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Other Project Cost (OPC)			
FY 2016	5,000	5,000	1,430
FY 2017	5,000	5,000	5,306
FY 2018	14,000	14,000	11,699
FY 2019	2,000	2,000	1,863
FY 2020	2,000	2,000	963
Outyears	–	–	6,739
Total, OPC	**28,000**	**28,000**	**28,000**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Project Cost (TPC)			
FY 2016	5,000	5,000	1,430
FY 2017	5,000	5,000	5,306
FY 2018	30,000	30,000	11,699
FY 2019	62,000	62,000	23,917
FY 2020	62,000	62,000	37,584
FY 2021	62,000	62,000	74,146
FY 2022	75,100	75,100	75,000
Outyears	288,900	288,900	360,918
Total, TPC	**590,000**	**590,000**	**590,000**

4. Details of Project Cost Estimate

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design	95,702	69,800	**N/A**
Design - Contingency	40,009	19,950	**N/A**
Total, Design (TEC)	**135,711**	**89,750**	**N/A**
Equipment	300,615	230,400	**N/A**
Construction - Contingency	125,674	60,050	**N/A**
Total, Construction (TEC)	**426,289**	**290,450**	**N/A**
Total, TEC	**562,000**	**380,200**	**N/A**
Contingency, TEC	*165,683*	*80,000*	***N/A***
Other Project Cost (OPC)			
R&D	8,200	8,000	**N/A**
Conceptual Planning	2,000	2,000	**N/A**
Conceptual Design	12,100	12,100	**N/A**
Start-up	2,000	2,000	**N/A**
OPC - Contingency	3,700	5,900	**N/A**
Total, Except D&D (OPC)	**28,000**	**30,000**	**N/A**
Total, OPC	**28,000**	**30,000**	**N/A**
Contingency, OPC	*3,700*	*5,900*	***N/A***
Total, TPC	**590,000**	**410,200**	**N/A**
Total, Contingency (TEC+OPC)	***169,383***	***85,900***	***N/A***

5. Schedule of Appropriations Requests

(dollars in thousands)

Request Year	Type	Prior Years	FY 2019	FY 2020	FY 2021	FY 2022	Outyears	Total
FY 2019	TEC	—	10,000	26,540	32,640	—	212,820	282,000
	OPC	10,000	2,000	5,000	—	—	21,000	38,000
	TPC	10,000	12,000	31,540	32,640	—	233,820	320,000
FY 2020	TEC	16,000	60,000	13,000	68,000	—	181,000	338,000
	OPC	24,000	2,000	2,000	—	—	2,000	30,000
	TPC	40,000	62,000	15,000	68,000	—	183,000	368,000
FY 2021	TEC	16,000	60,000	60,000	13,000	—	231,200	380,200
	OPC	24,000	2,000	2,000	—	—	2,000	30,000
	TPC	40,000	62,000	62,000	13,000	—	233,200	410,200
FY 2022	TEC	16,000	60,000	60,000	62,000	75,100	288,900	562,000
	OPC	24,000	2,000	2,000	—	—	—	28,000
	TPC	40,000	62,000	62,000	62,000	75,100	288,900	590,000

6. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy	FY 2029
Expected Useful Life	25 years
Expected Future Start of D&D of this capital asset	FY 2054

Related Funding Requirements
(dollars in thousands)

	Annual Costs		Life Cycle Costs	
	Previous Total Estimate	**Current Total Estimate**	**Previous Total Estimate**	**Current Total Estimate**
Operations, Maintenance and Repair	N/A	—	N/A	—

7. D&D Information

At this stage of project planning and development, SC anticipates that there will be no new area being constructed in the construction project.

8. Acquisition Approach

DOE has determined that the Lawrence Berkeley National Laboratory (LBNL) will acquire the ALS-U project under the existing DOE Management and Operations (M&O) contract.

LBNL provided a Preliminary Design Report for the ALS-U project and identified key design activities, requirements, and high-risk subsystem components 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 LBNL-wide resource.

LBNL may partner with other laboratories for design and procurement of key technical subsystem components. Technical system designs will require research and development activities. Cost estimates for these systems are based on ALS actual costs and other similar facilities, to the extent practicable. Planning and budgeting for the project will exploit recent cost data from similar projects. LBNL or partner laboratory staff will complete the design of the technical systems. 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. The M&O contractor’s performance will be evaluated through the annual laboratory performance appraisal process.

Lessons learned from other SC projects and other similar facilities will be exploited fully in planning and executing ALS-U.

18-SC-13, Linac Coherent Light Source-II-High Energy (LCLS-II-HE), SLAC
SLAC National Accelerator Laboratory
Project is for Design and Construction

1. Summary, Significant Changes, and Schedule and Cost History

Summary
The FY 2022 Request for the Linac Coherent Light Source-II High Energy (LCLS-II-HE) project is $50,000,000 of Total Estimated Cost (TEC) funding and $3,000,000 of Other Project Costs (OPC). The most recent DOE Order 413.3B approved Critical Decision (CD) is CD-3A, Approve Long-Lead Procurements, which was approved on May 12, 2020. This project at CD-1 established a preliminary Total Project Cost (TPC) range of $290,000,000 to $480,000,000. This cost range encompassed the most feasible preliminary alternatives at CD-1. The CD-1 preliminary TPC point estimate for this project was $368,000,000. Pending CD-2 reviews, the project's current TPC estimate is $660,000,000.

Significant Changes
The LCLS-II HE project was initiated in FY 2019. The project's Total Project Cost (TPC) estimate has increased from $428,000,000 to $660,000,000 between CD-3A and the current budget request as a result of a maturing design effort that identified additional costs across the project scope, added scope for a new superconducting electron source, and increased contingency to address several future risks. A major risk concerns the ability to operate the LCLS-II cryomodules above their design accelerating gradient and their ability to meet their design operating gradient, which is significantly higher than previously achieved with current technology. The R&D program in progress for the LCLS-II-HE cryomodules has shown promise and is nearly complete. Due to delays caused by the coronavirus pandemic (COVID-19), the performance of the LCLS-II cryomodules will not be known until sometime in FY 2022 when the LCLS-II project begins the accelerator commissioning. Both risks can be mitigated by adding additional cryomodules to the project at additional cost. The LCLS-II-HE project is currently assessing the impact of COVID-19 on the project's cost, schedule, and project milestones. The combined CD-2/3 approval is now projected for 4Q FY 2022 and CD-4 is now projected for 2Q FY 2030.

FY 2020 funding continued the support of planning, engineering, design, R&D prototyping, and long-lead procurements. FY 2021 funding continues engineering, design, R&D, prototyping, and long-lead procurements of construction items. FY 2022 funding will support engineering, design, R&D, prototyping, continuing long-lead procurements, and preparations for baselining the project.

A Federal Project Director, certified to Level IV, has been assigned to this project and has approved this CPDS.

Critical Milestone History

Fiscal Year	CD-0	Conceptual Design Complete	CD-1	CD-2	Final Design Complete	CD-3	D&D Complete	CD-4
FY 2019	12/15/16	3Q FY 2019	1Q FY 2019	1Q FY 2021	1Q FY 2023	2Q FY 2022	N/A	2Q FY 2026
FY 2020	12/15/16	3/23/18	9/21/18	2Q FY 2023	1Q FY 2023	2Q FY 2023	N/A	1Q FY 2028
FY 2021	12/15/16	3/23/18	9/21/18	2Q FY 2023	1Q FY 2023	2Q FY 2023	N/A	1Q FY 2029
FY 2022	12/15/16	3/23/18	9/21/18	4Q FY 2022	3Q FY 2022	4Q FY 2022	N/A	2Q FY 2030

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 Alternative Selection and Cost Range
CD-2 – Approve 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

Fiscal Year	Performance Baseline Validation	CD-3A
FY 2019	1Q FY 2021	4Q FY 2019
FY 2020	2Q FY 2023	4Q FY 2019
FY 2021	2Q FY 2023	2Q FY 2020
FY 2022	4Q FY 2022	5/12/20

CD-3A – Approve Long-Lead Procurements for cryomodule associated parts and equipment.

Project Cost History

(dollars in thousands)

Fiscal Year	TEC, Design	TEC, Construction	TEC, Total	OPC, Except D&D	OPC, D&D	OPC, Total	TPC
FY 2019	34,000	266,000	300,000	20,000	N/A	20,000	320,000
FY 2020	34,000	314,000	348,000	20,000	N/A	20,000	368,000
FY 2021	34,000	374,000	408,000	20,000	N/A	20,000	428,000
FY 2022	39,000	589,000	628,000	32,000	N/A	32,000	660,000

2. Project Scope and Justification

Scope

The LCLS-II-HE project's scope includes increasing the superconducting linac energy from 4 giga-electronvolts (GeV) to 8 GeV by installing additional cryomodules in the first kilometer of the existing linac tunnel. The electron beam will be transported to the existing undulator hall to extend the x-ray energy to 12 keV and beyond. The project will also modify or upgrade existing infrastructure and x-ray transport, optics and diagnostics system, and provide new or upgraded instrumentation to augment existing and planned capabilities. Recently added scope includes a new, superconducting electron source and increased contingency to address several future risks. Additional scope is being considered to address several risks associated with the linac performance, operation reliability and scientific mission capability.

Justification

The leadership position of LCLS-II will be challenged by the European x-ray free electron laser (XFEL) at DESY in Hamburg, Germany, which began operations in 2017. The European XFEL has a higher electron energy, which allows production of shorter (i.e., harder) x-ray wavelength pulses compared to LCLS-II. More recent plans emerging from DESY have revealed how the European XFEL could be extended from a pulsed operation mode to continuous operation, which would create a profound capability gap compared to LCLS-II. The continuous operation improves the stability of the electron beam and provides uniformly spaced pulses of x-rays or, if desired, the ability to customize the sequence of x-ray pulses provided to experiments to optimize the measurements being made.

In the face of this challenge to U.S. scientific leadership, extending the energy reach of x-rays beyond the upper limit of LCLS-II (5 keV) is a high priority. 12 keV x-rays correspond to an x-ray wavelength of approximately 1 Ångstrom, which is particularly important for high resolution structural determination experiments since this is the characteristic distance between bound atoms in matter. Expanding the photon energy range beyond 5 keV will allow U.S. researchers to probe earth-abundant elements that will be needed for large-scale deployment of photo-catalysts for electricity and fuel production; it allows the study of strong spin-orbit coupling that underpins many aspects of quantum materials; and it reaches the biologically important selenium k-edge, used for protein crystallography.

There is also a limited ability to observe and understand the structural dynamics of complex matter at the atomic scale with hard x-rays, at ultrafast time scales, and in operational environments. Overcoming this capability gap is crucial for the design, control and understanding of new advanced materials necessary to develop new energy technologies. To achieve this objective, the Department needs a hard x-ray source capable of producing high energy ultrafast bursts, with full spatial and temporal coherence, at high repetition rates. Possession of a hard x-ray source with a photon energy range from 5- 12 keV and beyond would enable spectroscopic analysis of additional key elements in the periodic table, deeper penetration into materials, and enhanced resolution. This capability cannot be provided by any existing or planned light source.

The LCLS-II project at SLAC, which is currently under construction and will begin operations in 2022-2024 is the first step to address this capability gap. LCLS-II will be the premier XFEL facility in the world at energies ranging from 200 eV up to approximately 5 keV. The cryomodule technology that underpins LCLS-II is a major advance from prior designs that will allow continuous operation up to 1 megahertz (MHz).

When completed, LCLS-II will be powered by SLAC's 4 GeV superconducting electron linear accelerator (linac). Over the past years, the cryomodule design for LCLS-II has performed beyond expectations, providing the technical basis to double the electron beam energy. It is therefore conceivable to add additional acceleration capacity at SLAC to double the electron beam energy from 4 GeV to 8 GeV. Calculations indicate that an 8 GeV linac will deliver a hard x-ray photon beam with peak energy of 12.8 keV, which will meet the mission need.

The LCLS-II-HE project will upgrade the LCLS-II to fully address the capability gaps and maintain U.S. leadership in XFEL science. The upgrade will provide world leading experimental capabilities for the U.S. research community by extending the x-ray energy of LCLS-II from 5 keV to 12 keV and beyond. The flexibility and detailed pulse structure associated with the proposed LCLS-II-HE facility will not be matched by other facilities under development worldwide.

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 facility is by upgrading the LCLS-II, currently under construction at SLAC, by increasing the energy of the superconducting accelerator and upgrading the existing infrastructure and instrumentation.

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

Key Performance Parameters (KPPs)

The Key Performance Parameters (KPPs) are preliminary and may change as the project continues towards CD-2. At CD-2 approval, the KPPs will be baselined. The Threshold KPPs represent the minimum acceptable performance that the project must achieve. The Objective KPPs represent the desired project performance. Achievement of the Threshold KPPs will be a prerequisite for approval of CD-4, Project Completion.

Performance Measure	Threshold	Objective
Superconducting linac electron beam energy	≥ 7 GeV	≥ 8 GeV
Electron bunch repetition rate	93 kHz	929 kHz
Superconducting linac charge per bunch	0.02 nC	0.1 nC
Photon beam energy range	200 to ≥ 8,000 eV	200 to ≥ 12,000 eV
High repetition rate capable, hard X-ray end stations	≥ 3	≥ 5
FEL photon quantity (10^{-3} BW)	$5x10^8$ (50x spontaneous @ 8 keV)	> 10^{11} @ 8 keV (200 μJ) or > 10^{10} @ 12.8 keV (20 μJ)

3. Financial Schedule

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Estimated Cost (TEC)			
Design (TEC)			
FY 2018	2,000	2,000	–
FY 2019	10,000	10,000	130
FY 2020	8,000	8,000	2,884
FY 2021	8,000	8,000	8,000
FY 2022	6,000	6,000	12,000
Outyears	5,000	5,000	15,986
Total, Design (TEC)	**39,000**	**39,000**	**39,000**
Construction (TEC)			
FY 2018	6,000	6,000	–
FY 2019	15,200	15,200	4,270
FY 2020	25,457	25,457	19,620
FY 2021	44,000	44,000	32,000
FY 2022	44,000	44,000	70,000
Outyears	454,343	454,343	463,110
Total, Construction (TEC)	**589,000**	**589,000**	**589,000**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Estimated Cost (TEC)			
FY 2018	8,000	8,000	–
FY 2019	25,200	25,200	4,400
FY 2020	33,457	33,457	22,504
FY 2021	52,000	52,000	40,000
FY 2022	50,000	50,000	82,000
Outyears	459,343	459,343	479,096
Total, TEC	**628,000**	**628,000**	**628,000**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Other Project Cost (OPC)			
FY 2018	2,000	2,000	1,191
FY 2019	6,000	6,000	2,041
FY 2020	4,000	4,000	4,081
FY 2021	2,000	2,000	3,000
FY 2022	3,000	3,000	4,000
Outyears	15,000	15,000	17,687
Total, OPC	**32,000**	**32,000**	**32,000**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Project Cost (TPC)			
FY 2018	10,000	10,000	1,191
FY 2019	31,200	31,200	6,441
FY 2020	37,457	37,457	26,585
FY 2021	54,000	54,000	43,000
FY 2022	53,000	53,000	86,000
Outyears	474,343	474,343	496,783
Total, TPC	**660,000**	**660,000**	**660,000**

Note – In FY 2021, the Office of Science reprogrammed $19,343,211.24 of prior year funds to the LCLS-II project at SLAC. The Prior Year Budget Authority in the table above reflects this reprogramming and additional funds are included in the outyears to maintain the project profile.

4. **Details of Project Cost Estimate**

	(dollars in thousands)		
	Current Total Estimate	**Previous Total Estimate**	**Original Validated Baseline**
Total Estimated Cost (TEC)			
Design	35,000	30,500	**N/A**
Design - Contingency	4,000	3,500	**N/A**
Total, Design (TEC)	**39,000**	**34,000**	**N/A**
Site Preparation	8,000	3,000	**N/A**
Equipment	410,000	250,700	**N/A**
Other Construction	29,000	9,000	**N/A**
Construction - Contingency	142,000	111,300	**N/A**
Total, Construction (TEC)	**589,000**	**374,000**	**N/A**
Total, TEC	**628,000**	**408,000**	**N/A**
Contingency, TEC	*146,000*	*114,800*	***N/A***
Other Project Cost (OPC)			
R&D	12,000	4,000	**N/A**
Conceptual Planning	2,000	1,500	**N/A**
Conceptual Design	2,000	2,000	**N/A**
Start-up	8,000	6,500	**N/A**
OPC - Contingency	8,000	6,000	**N/A**
Total, Except D&D (OPC)	**32,000**	**20,000**	**N/A**
Total, OPC	**32,000**	**20,000**	**N/A**
Contingency, OPC	*8,000*	*6,000*	***N/A***
Total, TPC	**660,000**	**428,000**	**N/A**
Total, Contingency (TEC+OPC)	***154,000***	***120,800***	***N/A***

5. Schedule of Appropriations Requests

(dollars in thousands)

Request Year	Type	Prior Years[a]	FY 2020	FY 2021	FY 2022	Outyears	Total
FY 2019	TEC	5,000	20,060	25,000	—	249,940	300,000
	OPC	2,000	4,000	—	—	14,000	20,000
	TPC	7,000	24,060	25,000	—	263,940	320,000
FY 2020	TEC	36,000	14,000	60,000	—	238,000	348,000
	OPC	8,000	4,000	—	—	8,000	20,000
	TPC	44,000	18,000	60,000	—	246,000	368,000
FY 2021	TEC	36,000	50,000	14,000	—	308,000	408,000
	OPC	8,000	4,000	2,000	—	6,000	20,000
	TPC	44,000	54,000	16,000	—	314,000	428,000
FY 2022	TEC	33,200	33,457	52,000	50,000	459,343	628,000
	OPC	8,000	4,000	2,000	3,000	15,000	32,000
	TPC	41,200	37,457	54,000	53,000	474,343	660,000

Note – In FY 2021, the Office of Science reprogrammed $19,343,211.24 of prior year funds to the LCLS-II project at SLAC. The FY 2022 Request in the table above reflects this reprogramming and additional funds are included in the outyears to maintain the project profile.

6. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy	FY 2030
Expected Useful Life	25 years
Expected Future Start of D&D of this capital asset	FY 2055

Related Funding Requirements
(dollars in thousands)

	Annual Costs		Life Cycle Costs	
	Previous Total Estimate	Current Total Estimate	Previous Total Estimate	Current Total Estimate
Operations, Maintenance and Repair	N/A	21,500	N/A	537,500

The numbers presented are the incremental operations and maintenance costs above the LCLS-II facility without escalation. The estimate will be updated and additional details will be provided after CD-2, Approve Project Performance Baseline.

7. D&D Information

At this stage of project planning and development, SC anticipates that there will be no new area being constructed in the construction project.

[a] While no funding was requested, Congress appropriated $10,000,000 for LCLS-II-HE in FY 2018.

8. Acquisition Approach

DOE has determined that the SLAC National Accelerator Laboratory will acquire the LCLS-II-HE project under the existing DOE Management and Operations (M&O) contract.

SLAC has prepared a Conceptual Design Report for the LCLS-II-HE project and has started preliminary design activities, identifying requirements and high-risk subsystem components 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 will partner with other 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-II and other similar facilities, to the extent practicable. The M&O contractor will fully exploit recent cost data in planning and budgeting for the project. SLAC or partner laboratory staff will complete the design of the technical systems. SLAC or subcontracted vendors with the necessary capabilities will fabricate the technical equipment. All subcontracts will be competitively bid and awarded based on best value to the government. The M&O contractor's performance will be evaluated through the annual laboratory performance appraisal process.

Lessons learned from the LCLS-II project and other similar facilities will be exploited fully in planning and executing LCLS-II-HE.

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

1. Summary, Significant Changes, and Schedule and Cost History

Summary

The FY 2022 Request is $32,400,000 including $28,100,000 in Total Estimated Cost funds and $4,300,000 in Other Project Costs funds. Following a baseline change in FY 2021, the Total Project Cost (TPC) is $1,136,400,000.

The most recent DOE Order 413.3B approved Critical Decisions (CD) are CD-2/3, Approve Performance Baseline and Approve Start of Construction, that were approved on March 21, 2016. A Baseline Change Proposal (BCP) was approved on October 13, 2020, by the Project Management Executive.

Significant Changes

This Construction Project Data Sheet (CPDS) is an update of the FY 2019 CPDS and does not include a new start for the budget year. The project was impacted by the coronavirus (COVID-19) pandemic which caused a baseline deviation. The new CD-4 milestone is projected for January 2024.

FY 2021 funding was used to continue the installation of all major accelerator and x-ray systems and equipment commissioning activities that were halted due to the COVID-19 Shelter in Place order issued by the local and state authorities on March 16, 2020. FY 2022 funding will support the completion of installation and commissioning activities for the project. The remaining work will follow all appropriate COVID-19 protocols and procedures to ensure the safety and health of project and subcontractor staff.

A Federal Project Director, certified to level IV, has been assigned to this project and has approved this CPDS.

Critical Milestone History

Fiscal Year	CD-0	Conceptual Design Complete	CD-1	CD-2	Final Design Complete	CD-3	D&D Complete	CD-4
FY 2013	4/22/10	-	10/14/11	1Q FY 2013	4Q FY 2016	3Q FY 2013	N/A	4Q FY 2019
FY 2014	4/22/10	-	10/14/11	4Q FY 2013	4Q FY 2016	4Q FY 2013	N/A	4Q FY 2019
FY 2015	4/22/10	-	10/14/11	4Q FY 2015	4Q FY 2017	4Q FY 2016	N/A	4Q FY 2021
FY 2016	4/22/10	1/21/14	8/22/14	2Q FY 2016	4Q FY 2017	2Q FY 2016	N/A	4Q FY 2021
FY 2017	4/22/10	1/21/14	8/22/14	2Q FY 2016	4Q FY 2017	2Q FY 2016	N/A	3Q FY 2022
FY 2018	4/22/10	1/21/14	8/22/14	3/21/16	4Q FY 2017	3/21/16	N/A	3Q FY 2022
FY 2019	4/22/10	1/21/14	8/22/14	3/21/16	4Q FY 2018	3/21/16	N/A	3Q FY 2022
FY 2020	4/22/10	1/21/14	8/22/14	3/21/16	4Q FY 2018	3/21/16	N/A	3Q FY 2022
FY 2021	4/22/10	1/21/14	8/22/14	3/21/16	4Q FY 2018	3/21/16	N/A	2Q FY 2024
FY 2022	4/22/10	1/21/14	8/22/14	3/21/16	9/28/18	3/21/16	N/A	2Q FY 2024

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 Alternative Selection and Cost Range
CD-2 – Approve 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

Fiscal Year	Performance Baseline Validation	CD-3A	CD-3B
FY 2013	1Q FY 2013	3/14/12	-
FY 2014	4Q FY 2013	3/14/12	-
FY 2015	4Q FY 2015	3/14/12	-
FY 2016	2Q FY 2016	3/14/12	3Q FY 2015
FY 2017	2Q FY 2016	3/14/12	5/28/15
FY 2018	3/21/16	3/14/12	5/28/15
FY 2019	3/21/16	3/14/12	5/28/15
FY 2020	3/21/16	3/14/12	5/28/15
FY 2021	3/21/16	3/14/12	5/28/15
FY 2022	3/21/16	3/14/12	5/28/15

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

Project Cost History

(dollars in thousands)

Fiscal Year	TEC, Design	TEC, Construction	TEC, Total	OPC, Except D&D[a]	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	47,000	946,100	993,100	51,900	N/A	51,900	1,045,000
FY 2018	47,000	946,100	993,100	51,900	N/A	51,900	1,045,000
FY 2019	47,000	946,100	993,100	51,900	N/A	51,900	1,045,000
FY 2020	47,000	946,100	993,100	51,900	N/A	51,900	1,045,000
FY 2021	47,000	1,033,200	1,080,200	59,800	N/A	59,800	1,140,000
FY 2022	47,000	1,033,200	1,080,200	56,200	N/A	56,200	1,136,400

[a] Other Project Costs (OPC) are funded through laboratory overhead.

2. 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 ten 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 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 three kilometer linac is being used to operate the LCLS facility, and the first two 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 feet.

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 1-25 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 $8,200,000. The construction costs were included in the Total Project Cost of $1,045M, and are maintained in the revised BCP Total Project Cost of $1,136.4M.

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 Order 413.3B, Program and Project Management for the Acquisition of Capital Assets.

Key Performance Parameters (KPPs)

The Threshold KPPs, 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.

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

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

Performance Measure	Threshold	Objective
FEL photon quantity (10^{-3} BW[a])	10^{10} (lasing @ 15,000 eV)	> 10^{12} @ 15,000 eV

3. Financial Schedule

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Estimated Cost (TEC)			
Design (TEC)			
FY 2012	2,000	2,000	2,000
FY 2013	5,000	5,000	5,000
FY 2014	4,000	4,000	2,040
FY 2015	21,000	21,000	9,089
FY 2016	15,000	15,000	20,500
FY 2017	–	–	6,040
FY 2018	–	–	2,331
Total, Design (TEC)	**47,000**	**47,000**	**47,000**
Construction (TEC)			
FY 2006	277	277	–
FY 2008	158	158	–
FY 2012	42,503	20,003	13,862
FY 2013	18,544	41,044	33,423
FY 2014	71,798	71,798	28,929
FY 2015	117,704	117,704	65,897
FY 2016	185,372	185,372	125,476
FY 2017	190,000	190,000	224,606
FY 2018	192,100	192,100	209,060
FY 2019	134,300	134,300	159,240
FY 2020	16,543	16,543	65,166
FY 2021	35,801	35,801	65,000
FY 2022	28,100	28,100	38,000
Outyears	–	–	4,541
Total, Construction (TEC)	**1,033,200**	**1,033,200**	**1,033,200**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Estimated Cost (TEC)			
FY 2006	277	277	–
FY 2008	158	158	–
FY 2012	44,503	22,003	15,862
FY 2013	23,544	46,044	38,423
FY 2014	75,798	75,798	30,969
FY 2015	138,704	138,704	74,986
FY 2016	200,372	200,372	145,976
FY 2017	190,000	190,000	230,646
FY 2018	192,100	192,100	211,391
FY 2019	134,300	134,300	159,240
FY 2020	16,543	16,543	65,166
FY 2021	35,801	35,801	65,000
FY 2022	28,100	28,100	38,000
Outyears	–	–	4,541
Total, TEC	**1,080,200**	**1,080,200**	**1,080,200**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Other Project Cost (OPC)			
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	–	–	116
FY 2014	10,000	10,000	8,581
FY 2015	9,300	9,300	2,660
FY 2016	–	–	34
FY 2017	–	–	758
FY 2018	7,900	7,900	2,204
FY 2019	6,100	6,100	3,038
FY 2020	–	–	3,545
FY 2021	–	–	5,500
FY 2022	4,300	4,300	6,500
Outyears	–	–	5,400
Total, OPC	**56,200**	**56,200**	**56,200**

(dollars in thousands)			
	Budget Authority (Appropriations)	**Obligations**	**Costs**
Total Project Cost (TPC)			
FY 2006	277	277	–
FY 2008	158	158	–
FY 2010	1,126	1,126	938
FY 2011	9,474	9,474	8,033
FY 2012	52,503	30,003	24,755
FY 2013	23,544	46,044	38,539
FY 2014	85,798	85,798	39,550
FY 2015	148,004	148,004	77,646
FY 2016	200,372	200,372	146,010
FY 2017	190,000	190,000	231,404
FY 2018	200,000	200,000	213,595
FY 2019	140,400	140,400	162,278
FY 2020	16,543	16,543	68,711
FY 2021	35,801	35,801	70,500
FY 2022	32,400	32,400	44,500
Outyears	–	–	9,941
Total, TPC	**1,136,400**	**1,136,400**	**1,136,400**

Note – In FY 2021, the Office of Science reprogrammed $23,199,000 of prior year funds and $2,801,000 of FY 2021 funds to the LCLS-II project at SLAC. The Budget Authority in the table above reflects this reprogramming.

4. **Details of Project Cost Estimate**

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design	47,000	47,000	42,125
Design - Contingency	N/A	N/A	4,875
Total, Design (TEC)	**47,000**	**47,000**	**47,000**
Site Preparation	24,700	24,700	24,700
Equipment	902,100	902,100	678,205
Other Construction	76,471	76,471	58,500
Construction - Contingency	29,929	29,929	184,695
Total, Construction (TEC)	**1,033,200**	**1,033,200**	**946,100**
Total, TEC	**1,080,200**	**1,080,200**	**993,100**
Contingency, TEC	*29,929*	*29,929*	*189,570*
Other Project Cost (OPC)			
R&D	1,972	1,972	1,972
Conceptual Planning	1,980	1,980	1,980
Conceptual Design	23,408	23,408	23,408
Start-up	22,190	22,190	15,790
OPC - Contingency	6,650	10,250	8,750
Total, Except D&D (OPC)	**56,200**	**59,800**	**51,900**
Total, OPC	**56,200**	**59,800**	**51,900**
Contingency, OPC	*6,650*	*10,250*	*8,750*
Total, TPC	**1,136,400**	**1,140,000**	**1,045,000**
Total, Contingency (TEC+OPC)	***36,579***	***40,179***	***198,320***

5. Schedule of Appropriations Requests

(dollars in thousands)

Request Year	Type	Prior Years	FY 2020	FY 2021	FY 2022	Outyears	Total
FY 2012 (MIE)	TEC	22,000	TBD	TBD	TBD	TBD	TBD
	OPC	18,600	TBD	TBD	TBD	TBD	TBD
	TPC	40,600	TBD	TBD	TBD	TBD	TBD
FY 2013 (MIE)	TEC	385,000	—	—	—	—	385,000
	OPC	20,000	—	—	—	—	20,000
	TPC	405,000	—	—	—	—	405,000
FY 2014	TEC	385,000	—	—	—	—	385,000
	OPC	20,000	—	—	—	—	20,000
	TPC	405,000	—	—	—	—	405,000
FY 2015	TEC	846,400	—	—	—	—	846,400
	OPC	48,600	—	—	—	—	48,600
	TEC	895,000	—	—	—	—	895,000
FY 2016	TEC	916,400	—	—	—	—	916,400
	OPC	48,600	—	—	—	—	48,600
	TPC	965,000	—	—	—	—	965,000
FY 2017	TEC	993,100	—	—	—	—	993,100
	OPC	51,900	—	—	—	—	51,900
	TPC	1,045,000	—	—	—	—	1,045,000
FY 2018	TEC	993,100	—	—	—	—	993,100
	OPC	51,900	—	—	—	—	51,900
	TPC	1,045,000	—	—	—	—	1,045,000
FY 2019	TEC	993,100	—	—	—	—	993,100
	OPC	51,900	—	—	—	—	51,900
	TPC	1,045,000	—	—	—	—	1,045,000
FY 2020	TEC	993,100	—	—	—	—	993,100
	OPC	51,900	—	—	—	—	51,900
	TPC	1,045,000	—	—	—	—	1,045,000
FY 2021	TEC	993,100	—	—	—	—	993,100
	OPC	51,900	—	—	—	—	51,900
	TPC	1,045,000	—	—	—	—	1,045,000
FY 2022	TEC	999,756	16,543	35,801	28,100	—	1,080,200
	OPC	51,900	—	—	4,300	—	56,200
	TPC	1,051,656	16,543	35,801	32,400	—	1,136,400

Note – In FY 2021, the Office of Science reprogrammed $23,199,000 of prior year funds and $2,801,000 of FY 2021 funds to the LCLS-II project at SLAC. The FY 2022 Request in the table above reflects this reprogramming.

6. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy	FY 2024
Expected Useful Life	25 years
Expected Future Start of D&D of this capital asset	FY 2049

Related Funding Requirements
(dollars in thousands)

	Annual Costs		Life Cycle Costs	
	Previous Total Estimate	**Current Total Estimate**	**Previous Total Estimate**	**Current Total Estimate**
Operations	N/A	TBD	N/A	TBD
Utilities	N/A	TBD	N/A	TBD
Maintenance and Repair	N/A	TBD	N/A	TBD
Total, Operations and Maintenance	$38.6M	$38.6M	$1,317M	$1,317M

7. 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

8. Acquisition Approach

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

A Conceptual Design Report for the LCLS-II project was completed and was revised based on the new technical parameters. Key design activities, requirements, and high-risk subsystem components were 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.