The U.S. Department of Energy’s
Ten-Year-Plans for the
Office of Science National Laboratories
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INTRODUCTION

The Department of Energy (DOE) is responsible for the effective stewardship of 17 national laboratories, of those ten are stewarded by the Office of Science and focus on discovery science. The DOE national laboratories were created as a means to an end: victory in World War II and national security in the face of the new atomic age. Since then, they have consistently responded to national priorities: first for national defense, but also in the space race and more recently in the search for new sources of energy, new energy-efficient materials, new methods for countering terrorism domestically and abroad, and addressing important critical national needs.

Today, the national laboratories comprise the most comprehensive research system of their kind in the world. In supporting DOE’s mission and strategic goals, the SC national laboratories perform a pivotal function in the nation’s research and development (R&D) efforts: increasingly the most interesting and important scientific questions fall at the intersections of scientific disciplines—chemistry, biology, physics, astronomy, mathematics—rather than within individual disciplines. The SC national laboratories are specifically designed and structured to pursue research at these intersections. Their history is replete with examples of multi-and inter-disciplinary research with far-reaching consequences. This kind of synergy, and the ability to transfer technology from one scientific field to another on a grand scale, is a unique feature of SC national laboratories that is not well-suited to university or private sector research facilities because of its scope, infrastructure needs or multidisciplinary nature.

As they have pursued solutions to our nation’s technological challenges, the national laboratories have also shaped, and in many cases led, whole fields of science—high energy physics, solid state physics and materials science, nanotechnology, plasma science, nuclear medicine and radiobiology, and large-scale scientific computing, to name a few. This wide-ranging impact on the nation’s scientific and technological achievement is due in large part to the fact that since their inception the DOE national laboratories have been home to many of the world’s largest, most sophisticated research facilities. From the “atom smashers” which allow us to see back to the earliest moments of the Universe, to fusion containers that enable experiments on how to harness the power of the sun for commercial purposes, to nanoscience research facilities and scientific computing networks that support thousands of researchers, the national laboratories are the stewards of our country’s “big science.” As such, the national laboratories remain the best means the Laboratory knows of to foster multi-disciplinary, large-facility science to national ends.

In addition to serving as lynchpins for major laboratory research initiatives that support DOE missions, the scientific facilities at the SC national laboratories are also operated as a resource for the broader national research community. Collectively, the laboratories served over 30,000 facility users and more than 7,000 visiting scientists in Fiscal Year (FY) 2017, significant portions of which are from universities, other Federal agencies, and private companies.

DOE’s challenge is to ensure that these institutions are oriented to focus, individually and collectively, on achieving the DOE mission, that Government resources and support are allocated to ensure their long-term scientific and technical excellence, and that a proper balance exists among them between competition and collaboration.

This year, DOE engaged its laboratories in a strategic planning activity that asked the laboratory leadership teams to define an exciting, yet realistic, long-range vision for their respective institutions based on agreed-upon core
capabilities assigned to each. This information provided the starting point for discussions between the DOE leadership and the laboratories about the laboratories’ current strengths and weaknesses, future directions, immediate and long-range challenges, and resource needs, and for the development of a DOE plan for each laboratory. This document presents strategic plans for thirteen national laboratories for the period FY 2018-2027.

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1 A table depicting the distribution of core capabilities across the science and energy laboratories is provided in Appendix 1, along with the definitions for each core capability category. Appendix 2 provides a listing of the DOE missions.
AMES LABORATORY

Lab-at-a-Glance

Location: Ames, IA

Type: Single-program Laboratory

Contractor: Iowa State University of Science and Technology

Site Office: Ames Site Office

Website: www.ameslab.gov

FY 2016 Costs by Funding Source ($M)

- EERE $25.7
- BES $22.3
- Other SC $1.6
- FES $0.2
- BER $0.1
- ASCR $0.1
- Other DOE $2.2

Physical Assets:
- 10 acres and 13 buildings
- 340,968 GSF in buildings
- Replacement Plant Value: $88.6M
- 0 GSF in 0 Excess Facilities
- 0 GSF in 0 Leased Facilities

Human Capital:
- 303 Full Time Equivalent Employees (FTEs)
- 82 Joint Faculty
- 43 Postdoctoral Researchers
- 102 Graduate Student
- 83 Undergraduate Students
- 0 Facility Users
- 268 Visiting Scientists

Mission Overview

Ames Laboratory creates materials, inspires minds to solve problems, and addresses global challenges.

For 70 years, Ames Laboratory (AMES) has been a leader in the discovery, synthesis, analysis, and use of new materials. Born of precise and demanding syntheses, these new materials often display surprising and occasionally completely unexpected physical and chemical characteristics. Some of these materials revolutionized our understanding of the limits of responsiveness and functionality of human-made materials including giant magnetocaloric materials, metamaterials, high-temperature superconductors, photonic crystals, quasicrystals, topological materials, cooperative catalysts, and rare earths and their compounds.

AMES accelerates the discovery of new materials and explores their fundamental physics and chemistry, adds value by sharing these materials and its know-how with the scientific community and partners throughout the U.S. and the world, and advances and promotes the application of these materials for economic and national security. We characterize materials with specialty tools we develop and with world-leading capabilities at our Sensitive Instrument Facility. We bring value to the Department of Energy’s (DOE’s) scientific user facilities by performing challenging experiments that further advance their instrumentation. Through Strategic Partnership Projects, AMES advances our national and economic competiveness while reducing technical barriers for U.S. industry. We are a top national laboratory in converting science into licensed technologies.
Our dedication to DOE’s and our mission naturally inspires our scientists, engineers, and support staff. Our mission extends to inspiring the minds of undergraduate and graduate students—3,107 Masters and Ph.D. degrees have been awarded to students from Iowa State University, our contractor, based on their Ames Laboratory research.

Today, we are addressing the global challenge of critical materials as we lead DOE’s Critical Materials Energy Innovation Hub. And we are tackling the 100-year old technology of compressed vapor refrigeration to improve significantly efficiency and reliability through the CaloriCool™, part of DOE’s Energy Materials Network.

Building on our core capabilities, our vision is to lead the interdisciplinary science of accelerating the design, discovery, and fundamental understanding of advanced energy and chemical conversion materials through scientific and technical innovation and excellence in safety, operations, quality, and diversity.

Core Capabilities

Ames Laboratory’s core capabilities represent the greatest strengths of the laboratory that benefit the science needs of the Nation. Each of the three core capabilities identified by DOE’s Office of Science involves interdisciplinary teams of world-leading researchers that utilize unique expertise and capabilities to address areas of national need and deliver on DOE’s mission. Research is focused on transformational breakthroughs in the fundamental understanding of the physics and chemistry of materials using innovative approaches that arise from the core capabilities and unique strengths of the Laboratory. New fundamental discoveries in the core areas of Condensed Matter Physics and Materials Science, and Chemical and Molecular Science, enable successes in Applied Material Science and Engineering.

Ames Laboratory’s core capabilities support DOE’s strategic objectives, and those of DOE’s Office of Science, in particular, to

1. Deliver scientific discoveries, capabilities, and major scientific tools that transform the understanding of nature
2. Strengthen the connection between advances in fundamental science and technology innovation
3. Support a more economically competitive, secure, and resilient U.S. energy infrastructure.
4. Accelerate scientific breakthroughs and develop new innovations for more sustainable U.S. energy production, conversion, and usage.

1. Condensed Matter Physics and Materials Science

Ames Laboratory is a leader of condensed matter physics and materials science within the national scientific enterprise. Specifically, Ames Laboratory has been at the forefront of research in rare-earth science and novel electronic and magnetic materials since the Laboratory was started, seven decades ago. Ames Laboratory provides the Nation with the highest quality materials for conducting fundamental research, invents new materials, and provides key insights into the fundamental physics and chemistry of these materials. Ames Laboratory does this by working collaboratively both within the Laboratory and with external collaborators. It is the deep understanding that Ames Laboratory has in precision and demanding synthesis of the highest quality materials that allows the science community to disentangle the truly novel physics and chemistry from inherent impurity-caused materials issues that so frequently impact the scientific enterprise’s understanding of the nature of materials.

Ames Laboratory’s own research has revealed the complexities and intricacies of the phase diagram of the novel iron-superconductors and has charted the path for the scientific community to focus its effort
on new physics and emerging phenomena that help us understand high temperature superconductivity more broadly. Here Ames Laboratory’s research contributes in a cyclical fashion: synthesis, characterization, theory and modeling and back again. Ames Laboratory has a research culture with fully integrated feedback that has recently revealed novel topological electronic structures in Weyl semimetals (Nature Materials, DOI 10.1038/nmat4685) that are hoped to be a key element for next generation information systems enabled by quantum coherent states, indeed this is one of the opportunities outlined in the BES report “Challenges at the Frontiers of Energy and Matter”. Another of these challenges is atomic control of matter itself, and here Ames Laboratory has been leading the way in identifying synthesis methodologies that defy classical nucleation and reach an unusually high density of iron nano-islands on graphene (Journal of Applied Physics, DOI 10.1063/1.4973571). This advance is relevant to a wide range of materials useful for spin-enabled microelectronic devices and quantum computing, and provides a pathway to the ultimate goal of precisely controlling electron spins and electron coherence at the quantum level. Ames Laboratory has been able to grow bulk single crystals utilizing a broad range of techniques including constituents with high vapor pressures, high melting temperatures (Physical Review B, DOI 10.1103/PhysRevB.93.064509) and under hydrostatic pressures to address fundamental phenomena in highly correlated systems, magnetism, and superconductivity; while unraveling the complexity in stability and formation in intermetallic compounds. Designs of new engineered structures that can manipulate light in ways not seen in conventional materials have exhibited, for example, a strong magnetic response to wavelengths from the terahertz to infrared range (Nature Materials, DOI 10.1038/nmat4685). These new metamaterials could allow integration of terahertz optoelectronics with high-speed telecommunications.

Moving forward, Ames Laboratory is expanding the limits of computational methods for the scientific community by working on quantum Monte-Carlo simulations, self-consistent electronic structure calculations incorporating total energies, spin excitations spectra, and classical and quantum molecular-dynamics simulations. We are developing new algorithms to predict the structure and properties of complex materials. Pioneering theoretical methods with innovative-numerical algorithms are being created to enable computational discovery of new materials and to fashion materials by design using DOE’s significant leadership computing resources. These methods serve to guide experiments and reduce the time needed to develop advanced materials to serve the Nation’s energy needs.

While Ames Laboratory has developed science and capabilities to utilize the full palette of the periodic table to achieve its mission, it continues to develop the fundamental science and synthesis methods of rare-earth materials. From its unique facilities to produce, process, manipulate, and characterize rare-earth materials to the highly visible Basic Energy Science projects and applied programs such as the Critical Materials Institute (CMI) and CaloriCoolTM Consortium, all have benefited from and contributed to sustaining this key core capability. Basic research on rare earths at Ames Laboratory is distinguished by its strong tradition of inspiring and enabling novel energy technologies such as magnetostrictive actuators and magnetic refrigeration. The applications of rare earths have evolved rapidly over the years. While intuition, serendipity, and trial-and-error have been successful strategies in the past, modern demands for precise tuning and control require a clear theoretical basis and the mining of huge physico-chemical datasets.

**Primary Source of Funding:** Office of Science.

2. **Chemical and Molecular Science**

This core capability recognizes Ames Laboratory’s ability to develop and apply theoretical, computational, and experimental methods to study catalysts, chemical reactivity, energy conversion, metal and alloy surface dynamics, and biomimetic processes of benefit to expand the fundamental
understanding of the chemical of materials to ultimately provide new solutions to reduce energy demands of chemical production and processing.

Ames Laboratory improves the fundamental understanding of chemical processes for energy and security needs, and molecular design by utilizing and developing new simulation and modeling techniques. Ames Laboratory is globally recognized for its research focused at the interface between homogeneous and heterogeneous catalysis enabling the design of new catalysts that combine the best characteristics of both. New advances in catalysis are discovered at Ames Laboratory by using the secondary-functionalities to modify surface properties (e.g., the interaction with solvents, especially water) for the design of new types of heterogeneous catalytic systems. We have developed and applied in situ Raman imaging to measure the distribution of biomolecules important for energy capture within the plant tissue. We have also developed other chemical analysis tools that enable us to measure biological function in live plants with unprecedented spatial resolution. These significant breakthroughs were enabled by collaboration between synthesis, unique high-precision, high-sensitivity analytical tools, and close integration with theory. Fundamental research at Ames Laboratory has led to a non-toxic, plug-and-play replacement catalyst that works on a broad spectrum of feedstocks, even with impurities. Today, this catalyst is a commercial product and is used to produce high quality biodiesel fuel. The fundamental concepts developed and new understanding brought to light using characterization techniques developed at Ames Laboratory have led to new understanding of the role of synthesis methods in both hybrid catalyst design (Physical Chemistry and Chemical Physics, DOI 10.1039/c6cp07642d) and perovskite materials for solar cells (Chemistry of Materials, DOI 10.1021/acs.chemmater.6b01874).

Moving forward, Ames Laboratory interdisciplinary research teams are focused on understanding the chemical composition, reactivity, and dynamics at the interface of materials important for energy conversion including catalysts, solar conversion materials, metals and alloys, and biomaterials by developing and applying theoretical, computational, and experimental methods. Excelling at synthesis, in addition to computation, theory, and characterization of these materials is key. World-leading research enables the design of new catalysts that combine the best characteristics of both homogeneous and heterogeneous catalysts.

This capability provides the foundation needed for the discovery of new, advanced catalysts and the development of energy efficient processes for bio-, photo-, and thermal catalytic conversions of chemical feedstocks.

**Primary Source of Funding**: Office of Science.

### 3. Applied Materials Science and Engineering

The application of knowledge derived from fundamental experimental, computational, and theoretical research to invent, design, and synthesize advanced materials with specific energy- and environment-relevant functionalities is a well-known strength of the Laboratory. Ames Laboratory develops, demonstrates, qualifies, and deploys materials that accelerate technological advancements in a wide range of fields—from materials that keep things cool in the European Space Agency’s Planck satellite, to a lead-free solder used in virtually all electronics, to analytical techniques that can detect harmful chemicals at parts-per-trillion concentrations, to new materials for efficient electrical transmission.

Advances in fundamental science through Basic Energy Sciences (BES) funded research in extraordinarily responsive materials has motivated expansion into applied areas, such as sensors or cooling technologies with caloric materials, which are thermodynamically responsive but need better response and control. This research led to the creation in fiscal year (FY) 2016 of CaloriCoolTM, the caloric materials consortium, part of DOE’s Energy Materials Network (EMN). CaloriCoolTM is one of four consortia to accelerate innovation around the clean energy
industry’s most pressing materials challenges by designing, discovering, and deploying materials in which reversible, thermal (caloric) response is triggered by magnetic, stress, and electric fields, or any combination of these fields.

Ames Laboratory’s world-leading advanced powder processing capabilities are advancing rapid and low-loss additive manufacturing of metal and metal oxides. We have developed mechanisms for unprecedented control over particle size and voiding and scaling of nanocrystalline to bulk material while retaining the fine-scale microstructural features responsible for enhanced properties and performance with additive manufacturing. Ames Laboratory is filling a critical need in advancing fundamental knowledge of advanced manufacturing by solving several technical challenges for powder feedstock. This is being achieved through improved process yield, powder surface quality and passivation, and particle size/shape uniformity and yield to tailor feedstock for advanced manufacturing processing by gas atomization. Working with sister laboratories, Ames Laboratory is developing key tools and models to address key barriers to metal additive manufacturing. Ames Laboratory is also developing a sophisticated additive manufacturing testbed to enable rapid process development and informed qualification of the additive manufacturing components and processes.

This core capability is further strengthened by the highly successful Critical Materials Institute (cmi.ameslab.gov), a DOE Energy Innovation Hub, led by Ames Laboratory. The mission of the CMI is to assure supply chains of materials critical to clean energy technologies—enabling innovation in U.S. manufacturing and enhancing U.S. energy security. Rare-earth elements are the most prominent of the critical materials today. CMI’s efforts aim to assure economically viable processing techniques for improved availability of these materials for clean-energy technologies, develop new techniques to recover materials from waste and scrap, and find acceptable alternatives to critical materials for use in devices such as generators, motors, lighting, and magnets. In the first four years, CMI funded researchers have filed 31 patent applications, had 2 patents issued, and licensed two technologies.

With our applied research in decision sciences, we work to integrate models, information and other artifacts related to a product or process. We challenge the notion that one cannot integrate analysis into decision making on-the-fly. Ames Laboratory accelerates manufacturing via an integrated, virtual engineering design environment VE-Suite (www.VESuite.org). This package is open-source software that links models, process simulations, data and real-time graphics to permit 3-D, real-time engineering design of complex systems, like next-generation power plants, efficient cars, and video games. Two spin-off companies, Praxik (www.praxik.com) and AgSolver (www.agsolver.com), were created in 2013 to deploy interactive, visually based, decision-making environments based on this software.


Science Strategy for the Future

For 70 years, Ames Laboratory has been a leader in the discovery, synthesis, analysis, and use of new materials. Born of precise and demanding syntheses, these new materials often display surprising and occasionally completely unexpected physical and chemical characteristics. Some of these materials revolutionized our understanding of the limits of responsiveness and functionality of man-made materials including strongly correlated electron materials and novel superconductors, quasicrystals, chiral materials, topological materials, cooperative catalysts, powders for advanced manufacturing, and rare earths and their compounds amongst many others.

Building on its history of discovery and use-inspired science, today Ames Laboratory is a world-leading institution that:
• Invents new materials through creative and innovative syntheses techniques, which are aggressively developed and refined;
• Determines the physics and chemistry of these materials using instrumentation developed at Ames Laboratory as well as instrumentation available at the nation’s scientific user facilities;
• Shares these materials with partners, and collaborates nationwide and worldwide to advance fundamental knowledge in materials science; and
• Promotes the applications of these materials for economic and national security through in-house activities and external collaborations.

The scientific strategy of the 2017 Ames Laboratory Annual Lab Plan is based on our recent Strategic Plan, which describes important new directions and targets of opportunity in materials discovery that are needed for challenges in energy, information, next generation computing technologies, energy conversion, and energy harvesting technologies. Wherever possible we shall harvest these advances for applications in the real world. These scientific themes are based on our current strengths, a competitive analysis of the field, and the timeliness of the research based on the BES Basic Research Needs Workshops and the Transformative Challenges Report.

Infrastructure

Overview of Site Facilities and Infrastructure

Ames Laboratory is a Government-owned, contractor-operated facility located in Ames, Iowa on the campus of Iowa State University (ISU). There is no federally-owned land at the site (See the Ames Laboratory Land Use Plan). The Laboratory occupies 10 acres of land leased from the Iowa Board of Regents where 13 DOE-owned buildings reside (340,968 gross square feet, GSF). There are four research buildings, an administrative building, and eight support buildings on the campus.

In 2015, construction on the newest research building, the Sensitive Instrument Facility (SIF), which is a 13,304 GSF structure to house state-of-the-art transmission electron microscopes and other sensitive electronic equipment, was completed.

The three older research buildings (Wilhelm, Spedding, and Metals Development) on the main campus are 50-60 years old; they have good structural integrity though designed for research needs of the mid to late 1900s. Each building has a mixture of wet and dry laboratories, offices, and conference spaces. Metals Development has high bay space currently utilized by the Facilities and Engineering Services machine shop that could be repurposed for research activities. These three buildings were all rated “substandard” in the 2014 DOE Laboratory Operations Board (LOB) infrastructure survey. The remaining DOE-owned buildings are rated “adequate”. The Laboratory also utilizes ISU space for research and support. In 2016, the Laboratory leased 34,479 net usable square feet (NUSF) of university space. Co-location of staff resulted in ISU leasing 26,271 NUSF of Ames Laboratory space. Ames Laboratory has no utility generating plants; the Laboratory receives its utilities from Iowa State University and the City of Ames.

The four main research buildings are for general use and support research for all three of our core capabilities: (1) condensed matter physics and materials science, (2) chemical and molecular science, and (3) applied materials science and engineering. Our workforce includes approximately 750 people who work at Ames Laboratory as staff, students, or associates.
<table>
<thead>
<tr>
<th>Asset</th>
<th>Facility Use</th>
<th>Gross Square Feet (GSF)</th>
<th>Year Built</th>
<th>Overall Asset Condition</th>
<th>Poor Condition Space (SF)</th>
<th>Fair Condition Space (SF)</th>
<th>Electrical Systems</th>
<th>Plumbing Systems</th>
<th>HVAC Systems</th>
<th>Roof/ Exterior</th>
</tr>
</thead>
<tbody>
<tr>
<td>Campus Warehouse</td>
<td>General Storage</td>
<td>16,506</td>
<td>1966</td>
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<td>25,964</td>
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<td>Deficient</td>
<td>Deficient/ Deficient</td>
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<td>Shed 1</td>
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<td>20,167</td>
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<td>Asset</td>
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<td>Harley Wilhelm Hall (HWH)</td>
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</table>

**Campus Strategy**

![Site Map: Ames Laboratory Main Campus located on Iowa State University’s Main Campus](image1)

![Site Map: Ames Laboratory Sensitive Instrument Facility located at Iowa State University’s Applied Sciences Complex](image2)

Our guiding principles for ensuring the facilities of Ames Laboratory are mission ready are to provide:

- Modern facilities and infrastructure to support our core capabilities
- A safe and secure work environment
- Productive workspaces
- Good stewardship of our national, DOE, and contractor resources

Guided by these principles, our mission supports basic research in the discovery, design and development of energy-relevant materials; research to attain foundational advances in materials chemistry, physics, and materials science and engineering.
To bring our campus up to the standards of the guiding principles and enhance Ames Laboratory’s ability to provide quality research, we have developed the following strategy:

- Design Integrated Materials Laboratory building
- Modernize the existing campus
- Provide mission-enabling spaces
- Extend the life of existing buildings and infrastructure

**Current Gaps**

During our mission readiness process, identification of several gaps kept recurring for all three of our older research buildings.

The Laboratory identified electrical power as a critical gap. This includes the current electrical supply infrastructure and its capacity. There are components to the distribution system that are original and need replaced. In addition, we are at capacity on many floors as new electrical devices joined our research toolset. Funding came from Basic Energy Science-General Plant Project (BES-GPP) over the last three years to address the immediate needs of 4160V switchgear replacement for the complex, and the 120/208V electrical distribution upgrades in Spedding Hall. SLI- GPP provided additional resources to upgrade the electrical distribution systems in Wilhelm Hall and Metals Development. The Laboratory needs to add distribution panels to each floor of these two research buildings, update circuit breakers in MD and increase 480V capacity in HWH to provide the power capacity needed now and in the future.

*Building improvements* are needed that will improve the research—for example, new windows in Spedding Hall will improve the research spaces’ ability to provide an environment conducive for today’s research by cutting down on drafts, dust, fumes and other contaminants that infiltrate the building. An issue with replacing the windows is the caulking has silica and asbestos that will require additional costs to remediate. The HVAC system in Metals Development needs replacement; it is the system original to the building built in 1961. Roofs continue to be a problem area for the Laboratory. The Laboratory has scheduled replacement of the roof in the worst condition (MD) in FY 2018 utilizing maintenance and general services dollars. SPH and HWH also need new roofs. The built-up roofs on these buildings are 20-30 years old and all have active leaks. The leaks damage the buildings, raise potential for mold, and pose a risk to expensive research equipment. The three older research buildings also need tuck-pointing to extend the lives of their exteriors.
Another big gap is the condition of the research labs themselves. The 2014 LOB infrastructure survey identified 100,890 square feet of space in the older buildings as being in poor or fair condition. Many of these labs have fixtures that date back to the original construction, cabinets that are rusted and hard to operate, work surfaces pocked from chemical exposure, asbestos that requires removal, and lighting updated. The condition of these spaces is detrimental to morale and is a barrier to recruiting and retention. In FY 2016, the Laboratory invested overhead dollars to renovate 3,992 square feet of the lab space in poor and fair condition and scheduled another 4,375 square feet of lab space for renovation in FY 2017. Our capacity to renovate space with overhead dollars is approximately 4,000 square feet per year (average of $300/s.f.). With 90,740 square feet of lab space remaining in poor or fair condition, it would take the Laboratory approximately 23 years to bring the spaces up to standard.

The charts below show the progress made by the Laboratory at improving poor, fair and good space from 2014 through 2017. Most of the improvements have focused on poor and fair space. The Laboratory performs updates to good space when it allows for contiguous space for the research project. The second chart relates the improvements to their respective core competency that the space supports. Charts three and four show the total of each condition type by square footage and number of rooms and the related progress for poor, fair and good spaces. The Laboratory used the totals from the 2014 LOB survey on space for comparison purposes.
Electronic access control is another gap. Starting under the American Recovery and Reinvestment Act (ARRA), the Laboratory began a project to convert its door access from physical keys to electronic proximity card readers. Once the ARRA funds were exhausted, the Laboratory allocated GPP funds to continue to make progress in the conversion. All of the exterior doors, the property protection areas for the site, and the interior doors for two buildings were completed. This system gives the operations staff a greater amount of control of different access situations and helps to provide better safety, security and accountability for room use. However, most of the interior doors in Spedding Hall and Metals Development are still key access only, and require conversion to proximity card access.

Computational sciences infrastructure is a critical gap. Ames Laboratory mission requirements have placed tremendous strain on the available computational resources and space. The Laboratory’s strong and evolving Office of Science, Basic Energy Sciences research coupled with our leadership role in the CMI and CaloriCool™ (part of the EERE Energy Materials Network) and supporting roles in several other research endeavors have strained the Laboratory’s physical infrastructure and computational resources. We are currently at or very near maximum power utilization in our buildings and are using valuable experimental laboratories and office space to house clusters and servers.

Ames Laboratory requires mid-scale high performance computing (HPC) to execute its mission to create materials and energy solutions. The increased focus on using computing resources to support the BES mission as well as growth in complementary efforts are creating need for more staff, more space, and more computational resources.

Ames Laboratory’s core expertise is in the discovery, design, synthesis, processing, and characterization of new materials with novel properties for new energy technologies. The resources needed to support
this mission have moved from solely bench-top science to experiments guided by computational modeling and simulations as enabled by advances in computer capabilities and speed. Ames Laboratory has world-class theory groups for materials and chemistry research that develop novel theories, algorithms, and computational models to support our scientific breakthroughs. As needed, scientists successfully compete for time on leadership class computers at ORNL, LBNL and ANL to run their codes, such as Gordon and Windus in 2015 and 2016 (200 million processor-hours per year). However, the gap is growing between what the Ames Laboratory researchers need and what is available on-site. Currently, our researchers are hindered by the infrastructure limits on space, power, and cooling for HPC needs. Dedicated HPC systems allow quicker model code development, debugging, and scale up prior to use at leadership computing facilities and necessary local computation for programs that are inefficient for running on leadership computers.

Recent conversations with staff in the SC-DDFO’s office have led to the plan that Ames Laboratory will look at collaborating with other laboratories to meet computing facility infrastructure needs. We have made a few contacts and have started a discussion internally to determine our needs and the impact of such an arrangement. AMES will put planning for local computing facility resources on hold until these discussions are complete.

Integrated Materials Laboratory building: Both the strategic planning and mission readiness processes identified the need for flexible and specialized research spaces in order to accommodate our strategic plan objectives and initiative. Rapid changes to work process configurations are impossible in the three older research buildings.

Workspaces with fixed walls and utilities buried within vertical utility chases make changes difficult. The existing buildings are fine for a significant portion of our research efforts but space that is specialized and can be quickly adapted for a particular initiative and then quickly changed once we move on to a new initiative is needed. With the recent conclusion of our Laboratory Strategic Plan and the input from this Laboratory Planning forum we plan to start a facility programing process to more fully evaluate our facility needs for the next five to ten years and report back on our findings in the coming year.

**Investment Summary**

**Electrical Systems Upgrades:** The Laboratory started the electrical systems upgrade using the FY 2014 allotment of BES-GPP funds ($600K) and some of the FY 2015 BES-GPP funds ($400K) to complete the first and second phases. The Laboratory received $2,000K under the Science Laboratory Infrastructure-General Plant Project (SLI-GPP) funding for FY 2017 to start the electrical system upgrades in Harley Wilhelm Hall and Metals Development.

**Building Improvements:** As the buildings continue to age, their many systems need replacement in order to extend the life of the building. Some of these projects are primarily maintenance in nature and are under maintenance and general services funded through overhead. These include new roofs ($1,300K over 7 years), and tuck-pointing ($900K over 5 years). Other projects, capital in nature, have been included in the funding request of this plan. They include replacement of the Spedding Hall windows ($1,000K), and replacement of the HVAC system in Metals Development ($1,000K). We have included these projects as BES-GPP funding requests scheduled as shown on Laboratory Investments Table. Though these are of high importance, they are lower priority than the electrical upgrades. Failure to invest in building improvements will contribute to the further deterioration of the buildings and accelerate their obsolescence.

**Research Labs:** We have included requests for SLI-GPP funds in this plan to renovate and improve research space. Our capacity to renovate space with overhead dollars is only 4,000 square feet
per year. The level of SLI-GPP funding requested in conjunction with continued investment of overhead dollars will allow for an orderly upgrade of poor and fair condition space. We have requested SLI-GPP ($1,000K per year) in FYs 2021, 2022, 2025-2028 to upgrade the laboratories and research areas in poor and fair condition. These projects are critical to improve the ability of the Laboratory to support modern science, improve morale and attract quality scientists. Failure to invest in the research labs will erode our ability to perform research in those spaces, keep key personnel, and to attract new staff.

**Electronic Access Control:** This project will complete the conversion of all interior doors to electronic access for Spedding Hall and Metals Development. The estimated cost to complete this project is $3,000K. The Laboratory is requesting SLI-GPP funding to complete this project in FY 2018 ($1,000K), FY 2019 ($1,000K), and FY 2020 ($1,000). After the conversion is complete, we will have the opportunity to tie the system to our training management system. This will make sure employees have completed the appropriate training before they have access to the work areas. This project will also improve our ability to lock-down our facility in case of a security issue.

**Building Maintenance and Repair:** The maintenance program, funded from overhead dollars, consists of activities necessary to keep the existing inventory of facilities in good working order and extend their service lives. It includes regularly scheduled maintenance, corrective repairs, and periodic replacement of components over the service life of the facility. It also includes facility management, engineering, documentation, and oversight required to carry out these functions. The condition of the research buildings has been maintained even as they age beyond normal service life. The Laboratory anticipates that it will need to continue to operate in the older buildings over the 10-year window of this plan. Historically AMES has invested approximately 2.0% of Replacement Plant Value (RPV) per year into maintenance and repair activities. This level of resources has been able to control deferred maintenance in the buildings. However, the combination of limited capital improvements and aging facilities has placed a greater demand on maintenance resources. Just maintaining the condition of the facilities does not ensure that they will continue to meet the needs of research activities. Maintenance and repair expenditures need to increase in order to replace aging components and reduce deferred maintenance. For this reason, the Laboratory increased maintenance and repair funding to approximately 2.8% of RPV in FY 2016, and plans to sustain this level for the next 5 years.

**Integrated Materials Laboratory building:** The Laboratory will use the results of the strategic planning process nearly completed to update its facility needs and identify the type of specialized facilities it will include in its request for a new facility. Several initiatives proposed in the strategic plan will require space configured differently than currently available in existing space. We will spend the next few months developing the facility plan and contracting for assistance to conceptually design and program the facility.

The two most critical of the gaps at the Laboratory are the need for scientific computing space and the aging electrical systems. We will work with other laboratories to facilitate additional computing space. The Laboratory received funding for electrical improvements. The Laboratory will address building improvements, research labs condition, electronic access control, and building maintenance and repair next. To fill these gaps, the Laboratory is requesting to sustain funding levels of $1,000K per year in GPP-BES, and $1,000K per year in GPP-SLI over the 10-year duration of this plan. The Laboratory is also requesting that the new construction start listed under 2020 for SLI funding be left as a place holder until next year’s Lab Planning discussion to allow the Lab time to complete its programming effort for an Integrated Materials Laboratory to support the new Laboratory Strategic Plan.
ARGONNE NATIONAL LABORATORY

Lab-at-a-Glance

Location: DuPage County, IL
Type: Multi-program Laboratory
Contractor: UChicago Argonne, LLC
Site Office: Argonne Site Office
Website: www.anl.gov

FY 2016 Costs by Funding Source ($M)

Physical Assets:
- 1,517 acres and 157 buildings
- 5.0 million GSF in buildings
- Replacement Plant Value: $3.29B
- 55,656 GSF in 20 Excess Facilities
- 339k GSF in Leased Facilities

Human Capital:
- 3206 Full Time Equivalent Employees (FTEs)
- 256 Joint Faculty
- 268 Postdoctoral Researchers
- 322 Graduate and 260 Undergraduate Students
- 7,422 Facility Users
- 1,005 Visiting Scientists

Mission Overview

Argonne National Laboratory was founded as a chemistry, materials and nuclear engineering laboratory in 1946, as the successor to the Manhattan Project’s Metallurgical Laboratory. Since then, as part of the Department of Energy (DOE) network of national laboratories, Argonne has built on its original strengths and expanded its mission in response to national needs.

Today, Argonne serves America as a science and energy laboratory distinguished by the breadth of its research and development capabilities combined with a unique portfolio of experimental and computational user facilities. Located just outside Chicago, Argonne has been managed since its founding by The University of Chicago, one of the world’s preeminent research universities.

In its science program, Argonne delivers new knowledge not only in chemistry and materials, but also in nuclear and particle physics, mathematics, and earth science. This work is enriched by collaborations with University of Chicago researchers, reflected in joint efforts in fields such as cosmological physics and computational materials.

Argonne’s early-stage R&D in energy encompasses nuclear, chemical, materials, bioprocess and systems engineering and drives advances in reactors, energy generation and storage, electricity distribution, and

FY 2016 Costs by Funding Source ($M)
transportation systems. The Laboratory nurtures strong connections with industry to support transfer of new technology concepts to the private sector.

The Laboratory’s science and energy programs both support and benefit from Argonne’s integrated user facilities. Each year, Argonne is a nexus of research for 8000+ scientists and engineers from other institutions, whose work is advanced by access to the Laboratory’s research centers and user facilities and by collaborations with Argonne’s staff. Argonne opened its first user facility in 1981 and today operates the Advanced Photon Source, Center for Nanoscale Materials, Argonne Tandem Linear Accelerator System, Argonne Leadership Computing Facility, and Atmospheric Radiation Measurement Climate Research Facility - Southern Great Plains site, which together serve one of the largest user communities in the DOE complex.

Overview

Argonne National Laboratory’s broad base of expertise in science and engineering, which comprises 18 of the 24 core capabilities defined by the Department of Energy (DOE), is a powerful asset to meet key national needs for scientific and technological leadership. We use these capabilities to advance the missions of DOE, the Department of Homeland Security (DHS), and other agencies.

Our multifaceted research and development (R&D) portfolio enables our scientists and engineers to deliver groundbreaking discovery science and innovative solutions to critical challenges in energy, security, and infrastructure. The value of our work to the nation is enriched by our collaboration with universities, particularly the University of Chicago (UChicago), industry, and other DOE national laboratories.

Core Capability Descriptions

Our core capabilities, listed in Table 3.1 and summarized on the following pages, lie in basic research, early-stage applied R&D, and major facilities. The expertise of our scientists and engineers both supports, and is supported by, our suite of large-scale experimental facilities that also serve researchers from outside Argonne. Those foundational facilities include:

Four on our Illinois site: the Advanced Photon Source (APS), Argonne Tandem-Linac Accelerator System (ATLAS), Argonne Leadership Computing Facility (ALCF), and Center for Nanoscale Materials (CNM)

One in Oklahoma: the Atmospheric Radiation Measurement Climate Research Facility - Southern Great Plains (ARM-SGP) site

Table 3.1 Argonne National Laboratory core capabilities

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<tr>
<th>Accelerator science and technology</th>
<th>Condensed matter physics and materials science</th>
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<td>Advanced computer science, visualization, and data</td>
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<td>Applied materials science and engineering</td>
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<td>Applied mathematics</td>
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<td>Biological and bioprocess engineering</td>
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<td>Chemical engineering</td>
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<tr>
<td>Computational science</td>
<td>Systems engineering and integration</td>
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</table>
1. Accelerator science and technology

*Capability*

Argonne’s core capability in accelerator science and technology centers around APS, ATLAS, and the Argonne Wakefield Accelerator (AWA) and ranges from electron storage rings and x-ray sources to hadron linear accelerators and advanced accelerator technology. These mutually enhancing proficiencies are the foundation for our successful operation of a suite of facilities that support a broad range of scientific research; they also form the basis for developing enabling technologies for future research and facilities at Argonne and other institutions. The nearly 200 Argonne scientists and engineers who work in this field are recognized internationally for their expertise in:

- Modeling, design, and operation of photon sources, electron accelerators and storage rings, free electron laser seeding and oscillators, and insertion devices, particularly superconducting undulators. We have complementary expertise in beam diagnostics, stability and feedback systems, and vacuum system engineering. All of these capabilities underlie our plans to upgrade the APS.

- Generation, acceleration, and reliable delivery of high-intensity stable and rare-isotope ion beams serving nuclear physics research at ATLAS. We are supporting several DOE and worldwide accelerator initiatives using expertise gained at ATLAS over the past 30 years in linear accelerator design and modeling and in the design and development of state-of-the-art superconducting radio-frequency cavity systems for low-velocity ions. Our unique expertise and infrastructure for low-beta cavity production and testing and for cavity cleaning and processing are currently being used to support three major efforts: the pulse-lengthening cavity for the APS Upgrade project; cryomodule production for the SLAC National Accelerator Laboratory’s Linac Coherent Light Source (LCLS)-II, in work being done in collaboration with Fermilab; and the Proton Improvement Plan (PIP)-II project at Fermilab for its future accelerator-based neutrino program.

- Advancements in high-gradient, two-beam acceleration using dielectrically loaded structures, in support of high energy physics research. This work is centered at the AWA, a unique facility combining the world’s highest electron bunch charge produced by a photocathode gun with a state-of-the-art linear accelerator and beam instrumentation. We are currently using AWA to evaluate emittance-exchange and emittance manipulation techniques in support of future capabilities in photon science, such as the successor to the APS Upgrade. It also is open to the user community for general accelerator R&D and high-bunch-charge experiments.

- Areas vital to future colliders, including high-power radio frequency sources, generation and preservation of high-brightness beams, photo-injectors, collective beam instabilities, two-beam acceleration, and positron production. This research is synergistic with work being performed to improve performance of light sources and for national security applications.

- State-of-the-art accelerator computation: our advanced accelerator modeling code “elegant” is used by researchers at more than 200 institutions worldwide.

- Development of EPICS software tools and applications for distributed control systems for accelerators.

Because of these capabilities, Argonne is a key partner in the development and construction of DOE-supported facilities elsewhere, including LCLS-II, PIP-II, the Facility for Rare Isotope Beams at Michigan State University, and electron-ion collider concepts. These partnerships build upon our previous substantial contributions to the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory and to LCLS.

*Mission relevance and funding*
This core capability supports the broad DOE/SC mission to enhance the capabilities of its current accelerator-based scientific user facilities while driving development of next-generation user facilities. Current sponsors include DOE/SC-BES, -HEP, and -NP and DOE/NNSA.

2. Advanced computer science, visualization, and data

Capability

Argonne is a leader in computer science, visualization, and data; we are recognized for expertise in operating systems and runtime software, programming models, scientific software developer productivity, data storage and input/output, distributed systems, workflows, visualization, and data analysis. This leadership is critical to achieving DOE’s exascale computing objectives.

We will continue to enhance and promote this capability and will build up new capacity in these areas:

- Foundational computing architectures and algorithms for quantum and neuromorphic computing, with a focus on software and methods for science
- Automation of scientific discovery through machine learning, cloud computing, and high-performance computing; this includes platforms to support materials science, chemistry, systems biology, and cosmology, and services that can be applied other areas, such as advanced manufacturing and security
- New concepts and strategies for data capture, management, transport, and storage of data, focused on DOE applications, that leverage our work in visualization, analysis, and workflows
- New systems architectures for end-to-end computing, to enable progress from today’s sensing-analysis-simulation-reasoning-control approach to tomorrow’s fully automated science, leveraging our expertise in system software, distributed computing, and cloud computing

Examples of ways in which Argonne’s computer science enhances multiple disciplines include:

- Data analysis capabilities for APS, including data transfer infrastructure and services from APS to ALCF for real-time analysis, and novel active learning algorithms and new parallel algorithms and software for ptychographic imaging
- Development of novel wireless sensor networks for science: the Waggle project is enabling a new breed of reliable sensors for smart-city applications and sensor-driven environmental science, and the Array of Things project is deploying these sensors in Chicago
- A new version of NekCEM (an R&D100 award winner) that recently achieved a 40x GPU/CPU performance improvement and sustained this performance to the full size of the Cray Titan XK7 (16,384 GPUs)

Argonne-developed software is also tested and deployed at the National Energy Research Scientific Computing Center at Lawrence Berkeley National Laboratory and at the Oak Ridge Leadership Computing Facility. Production supercomputer systems worldwide use Argonne’s research software tools, and in exascale computer science, we are highly regarded for our development of operating system and runtime software. Argonne’s expertise in resilience covers multilevel checkpoint/restart, signal-analysis-based failure prediction, domino-effect-free fault-tolerant protocols, and use of data analytics to detect silent data corruption. We are also involved in managing and executing DOE’s research plan for exascale computing, and maintain partnerships with researchers in Japan and Europe.

Mission relevance and funding

This core capability supports the DOE/SC-ASCR mission to develop and deploy high-performance and leadership computing resources for science discovery. Additional current sponsors include DOE/ECP;
DOE/SC-BER and -BES; NIH; and NSF. Much of this additional funding supports co-design activities and interdisciplinary research partnerships with scientists in various application areas.

3. Applied materials science and engineering

   Capability

   The value chain for materials development includes invention, innovation, and commercialization. Each step is critical to gaining the full value of the intellectual capital developed through discovery science. Argonne applies internationally recognized expertise in materials development, synthesis, and processing to drive advances in energy storage, clean energy technology and manufacturing processes.

   This work leverages a unique combination of resources: applied and basic science teams from across the Laboratory; materials characterization at the APS and CNM; computational science using the ALCF; one-of-a-kind facilities for materials synthesis, fabrication, and testing; polyelectrolyte science and polymer synthesis expertise from the UChicago-Argonne Institute for Molecular Engineering (IME); and scale up of materials for energy storage and water purification in our DOE/EERE-funded Material Engineering Research Facility (MERF).

   Our applied materials science and engineering has produced more-efficient batteries, new solar panel designs, high-performance sponges for oil absorption, nanofiber magnets, high-performance lubricants, and improved nuclear energy fuels and materials. Ongoing work has shown promise for more-efficient nuclear fuel reprocessing, lighter-weight transportation alloys, and higher-performance superconducting materials for use in detectors, accelerators, energy transmission, and energy storage.

   Additionally, two Argonne collaborative centers, Argonne Design Works (ADW) and the Argonne Collaborative Center for Energy Storage Science (ACCESS), are facilitating maturation of those novel materials and their deployment to industry. We also partner with industry in a number of innovative manufacturing institutes, including PowerAmerica, Digital Manufacturing Design and Innovation Institute (DMDII), and Reducing Embodied-energy and Decreasing Emissions (REMADE).

   Argonne is a leader in creating innovative materials and developing scalable processes and advanced manufacturing techniques to produce and apply those materials. For example, we develop thin films and nanostructured materials, using both atomic layer deposition and enhanced vapor deposition, and extend those technologies to a variety of applications, including high-performance catalysts for the chemical industry, nuclear energy materials with enhanced performance and safety characteristics, more-efficient solar cells and solid-state lighting, and radio frequency energy harvesting and advanced communication devices. In other work, we develop ultracapacitor materials for transportation applications and membrane materials and systems for gas- and liquid-phase separation, for applications such as hydrogen production, carbon dioxide separation, biofuels processing, lithium metal manufacture, and water treatment and reuse.

   The MERF enables us to develop scalable processes and advanced manufacturing techniques for producing innovative materials in sufficient quantities for industrial testing and accurate cost modeling, thereby bridging the gap between bench-scale science and industrial implementation.

   Argonne’s nuclear materials work focuses on verifying the safety of current light-water reactors and developing new, high-performance materials that promise to improve the economics and further enhance safety of advanced reactors. This research leverages our capability to design and develop materials for extreme conditions and our nuclear engineering capability.

   Mission relevance and funding

   This core capability supports the missions of DOE and other federal and private-sector organizations in the areas of nuclear energy, energy efficiency, renewable energy, energy storage, and environmental stewardship. Current sponsors include ARPA-E, DOE/EERE, DOE/NE, DOE/NNSA, DOE/SC-BES, DARPA,
NRC, and a wide and growing range of industrial partners who produce critical materials to enhance American competitiveness and strengthen national security.

4. Applied mathematics

   Capability

   Argonne is recognized for broad-ranging foundational research in mathematical modeling, analysis, and algorithm development, implemented in scalable software for the world’s largest computing systems. We excel in the scalable solution of partial differential equations (PDEs), provide best-in-class expertise in automatic/algorithmic differentiation (AD), and are a recognized leader in mathematical optimization theory, modeling, algorithms, and software. Our strategy for the future emphasizes:

   - Implementing time- and energy-efficient PDE and optimization solvers for exascale architectures
   - Extending PDE solvers to provide rigorous local and global error estimates and controls
   - Combining AD, PDE, and optimization capabilities to support efficient solution of design
   - Applying expertise in numerical optimization and AD as building blocks for scalable machine learning
   - Expanding our expertise in machine learning, statistics, quantum algorithms and other strategic areas
   - Combining problem-solving approaches using machine learning, applied statistics, and mathematical optimization to enable the solution of multimodal inverse problems and the analysis of simulation and experimental data

Important recent advances in Argonne’s applied mathematics capabilities include:

   - New capabilities for implicit-explicit time integration with a posteriori error estimation, nested and hierarchical solvers for increased scalability, and advanced solution-transfer and problem-coupling algorithms to address multiphysics and multiscale applications
   - New algorithms and problem formulations that calibrate energy density functions in nuclear physics and support analysis of APS coherent x-ray diffraction images
   - Enhanced language support for Python and R in the ADOL-C tool, in order to provide AD capabilities for data analysis, statistics, and machine learning applications

Argonne’s advances in applied mathematics are captured in state-of-the-art software, including:

   - The Nek5000 and NekCEM software packages, which employ the spectral element method to efficiently solve large problems in computational fluid dynamics and computational electromagnetics
   - PETSc, used by hundreds of scientific applications, which provides scalable linear solvers, nonlinear solvers, and time integration methods for solving discretized PDEs
   - The OpenAD/F, ADIC, and Rapsodia tools for AD
   - MINOTAUR, which solves optimization problems with both discrete and continuous variables
   - Scalable solvers, such as TAO and PIPS, for optimization problems with billions of variables and constraints

This software portfolio makes it possible to answer a broad range of science and engineering questions, including how to operate and upgrade the power grid, how mantle convection affects the geological evolution of the planet, how to efficiently cool nuclear reactors, and how to design and operate gas distribution networks.
Mission relevance and funding

This core capability supports the DOE/SC-ASCR mission to develop and deploy high-performance and leadership computing resources for scientific discovery. Additional current sponsors include DOE/ECP, DOE/EERE, DOE/NE, DOE/OE, DOE/SC-BER, NIH, and NSF.

5. Biological and bioprocess engineering

Capability

Argonne’s bioprocess research determines the fundamental engineering mechanisms for biological energy capture and conversion at the molecular to unit-operation scale, and uses the results to develop first-principles bioengineering approaches that we then apply to meet technology challenges in energy, environment, and carbon sequestration. Argonne pioneers new approaches to biological and bioprocess engineering that combine synthetic biology and synthetic chemistry to create bio-materials with tuned, collaborative functionalities.

This capability takes distinctive advantage of the CNM and APS. CNM’s tools for imaging and manipulating genomes, cells, and processes over multiple scales are extensively leveraged for bioprocessing. The APS is used to determine the crystallographic structure of biological macromolecules and to characterize catalysts in thermochemical conversion processes: capabilities include bionanoprobe and micro-diffraction tools and facilities that use APS beamlines. In all, 17 APS beamlines are largely dedicated to biological sample analysis, more than at any other synchrotron in the world, and the planned APS Upgrade will significantly enhance capabilities to probe biological materials. These tools are complemented by our Advanced Protein Characterization Facility, which can produce and characterize tens of thousands of unique proteins each year, including their kinetic and thermodynamic properties.

We are pursuing the following strategic directions and investments in unique capabilities:

- Integration of hybrid nanoparticles with biological molecules
- Protein design for robust catalysis and modulation of functionality
- Directed molecular evolution approach for natural photosynthetic systems
- Catalyst separation and bioreactor designs and operations from bench to pilot scale
- Extraction and separation of biofuel candidates from bioreactors without disruption of bioprocesses
- Leadership of a consortium of eight national laboratories to bring cost-effective and high-performing bioprocess separations technologies to market faster

Through recent advances in biological and bioprocess engineering, we have demonstrated the abilities to engineer microbes for biofuels and bioproducts production and to engineer energy-converting proteins with radically altered function. This creates a capability to design microbes and microbial communities for energy-water research and provides a synthetic biology capability to link with our capabilities in bio-hybrid research programs in chemistry and materials. We are developing experimental and computational approaches to facilitate understanding, predictive modeling, and design of microorganisms and microbial communities across scales. This includes a deep understanding of potential novel enzymatic reactions and other enzyme functions. We leveraged these capabilities in our recent response to the DOE-SC/BER call for proposals in biosystems design, as well as in our work in the soil microbiome research scientific focus area.

Through the DOE-SC/BER KBase project, we are integrating these modeling and computational analysis capabilities, including metabolic modeling and cheminformatics to support bioengineering efforts for microbes, plants, and microbial communities. We are also now part of the DOE/EERE-
sponsored Agile Biofoundry project contributing to developing biomanufacturing technologies. Additionally, we are a leader in lifecycle and techno-economic analyses of bioenergy-related processes and in analysis of bioenergy system deployment impacts on soil carbon, water footprint, water quality, and landscape design.

**Mission relevance and funding**

This core capability supports the missions of DOE and other entities that seek to better understand plants and microbes to engineer them for bioenergy, carbon storage, and bioremediation. Current sponsors include DOE/EERE, DOE/SC-BER, national security agencies, and industry.

6. **Chemical and molecular science**

   **Capability**

   Our core capability in chemistry, a central science at Argonne, encompasses research in catalysis; solar and photosynthetic processes; heavy elements; interfacial science; gas-phase chemical physics; and atomic, molecular, and optical science (AMOS). A unifying theme across this diverse set of capabilities is precision in placement, separation, controlled reactivity, and characterization of atoms and molecules, ranging from the gas phase to the solid state. The computational, synthetic, and structural determination tools embodied in the ALCF, APS and CNM are major assets to this capability.

   Argonne’s catalysis research studies the interactions between molecular metal catalysts and metal oxide surfaces, with an emphasis on their reactivity with light alkanes. This innovative and distinctive research focuses on organometallic chemistry, using atomic layer deposition to synthesize new catalysts. Theoretical, experimental, and computational chemists collaborate in groundbreaking studies, and use state-of-the-art in situ APS tools to study catalysis under realistic operating conditions.

   Our solar and photosynthetic research focuses on three areas: understanding structural dynamics in photo-induced charge separation processes, developing capabilities for investigating steps in solar-to-fuels energy conversion, and investigating fundamental mechanisms for electron transfer and chemical energy conversion in photosynthesis. Our work has demonstrated that the combination of chemical synthesis with biological synthesis can create biomimetic hybrids with combined chemical and photosynthetic functionalities.

   Argonne’s heavy element chemistry research seeks to understand the fundamental science of liquid-liquid separation as the process used to extract, isolate and purify the actinides, lanthanides, and their fission products; we also seek to understand chemical trends within the 5f series and how they integrate and inform similar studies across the periodic table. This program will be moving into a new radiological facility in the Materials Design Laboratory that is now under construction at Argonne.

   Our interfacial science research leverages the capabilities of the APS to understand molecular-scale controls over structure and reactivity at liquid-solid interfaces. Geological materials provide mechanistic insights into the processes that effectively control geochemical transport related to the disposition of the by-products of energy consumption. The Center for Electrochemical Energy Sciences (CEES), which leverages our extensive experience in battery research, studies interfacial processes and novel chemistries in lithium-ion battery systems, with the application of state-of-the-art experimental and computational capabilities.

   Argonne is a world leader in gas-phase chemical physics research, particularly in the context of combustion chemistry. Theoretical and experimental efforts span a wide range of activities in thermochemistry, dynamics, kinetics, and modeling, including those relevant to internal combustion engines. Our experimental capabilities include several unique instruments for studies of spectroscopy, dynamics, and kinetics over a wide range of temperatures and pressures.
Our AMOS research is advancing the understanding of x-ray interactions with atoms, molecules, and clusters, with the APS, LCLS, and other light sources. High-repetition-rate lasers and x-ray spectroscopy are used to explore and control the photo-induced dynamics of solvated molecules. Theorists and computational scientists work together to better understand x-ray radiation damage in complex systems, a matter of importance for Argonne’s planned APS Upgrade.

Mission relevance and funding

This core capability supports the missions of DOE/SC-BES and other DOE/SC programs. Additional current sponsors include ARPA-E, DOD, and NASA.

7. Chemical engineering

Chemical engineering research at Argonne addresses the nation’s energy and security challenges by building on and informing basic energy research while developing transformational technologies for electrochemical energy storage and energy conversion. We are globally recognized for our lithium-ion battery work that integrates basic research, applied R&D, scale-up, engineering, modeling and battery testing.

Argonne’s battery programs provide a unique, integrated suite of capabilities within the DOE complex: applied materials science and engineering; basic materials R&D; and the ability to scale materials to a pre-pilot level, incorporate materials in commercial-grade cells and run them through multiple tests, and then analyze the materials down to the molecular scale. This set of chemical engineering capabilities is accessible to external organizations that are developing battery materials and chemistries.

We intend to significantly leverage and expand our chemical engineering capabilities through a major initiative to promote the science basis for manufacturing energy materials and technologies, by integrating a unique set of capabilities and facilities including our:

- Cell Analysis, Modeling and Prototyping (CAMP) facility
- Electrochemical Analysis and Diagnostics Laboratory (EADL)
- High-Throughput Research (HTR) Laboratory
- Materials Engineering Research Facility (MERF)

These facilities and capabilities allow researchers to design, fabricate, and engineer advanced batteries, creating prototype electrodes and cell systems; EERE provides full funding for the CAMP facility and MERF as well as most of the EADL’s funding. CAMP-manufactured cells enable realistic, consistent, and timely evaluation of candidate chemistries in a close-to-realistic industrial format. The EADL provides battery developers with performance evaluation of cells, modules, and battery packs that allows diagnostic analysis of battery components after use to identify mechanisms that limit battery life. The HTR Laboratory provides a set of robotic tools and reactor systems for rapid, highly automated, and parallel approaches to chemical synthesis and materials development, thereby accelerating discovery and optimization of new materials for catalysis, energy storage, fuel cells, solar energy, and nanoscale chemistry. Finally, the MERF allows researchers to explore the scale up of critical materials needed for battery development and prototyping.

In addition to our leadership in battery R&D, we are recognized for our work in development and demonstration of fuel cell technology. This multidisciplinary effort is developing advanced membranes, electrodes, and electrocatalysts that reduce the cost and improve the durability of fuel cells based on both solid oxide and polymer electrolyte membrane technologies. We also are accelerating the development of catalysts that do not use platinum group metals, by developing and using high-
throughput materials synthesis, characterization, and performance evaluation equipment and methodologies. This activity is a cornerstone of the Department of Energy’s ElectroCat research consortium, which is co-led by Argonne and Los Alamos National Laboratory.

**Mission relevance and funding**

This core capability supports the missions of DOE and other agencies to advance energy storage and fuel cell science and engineering. Current sponsors include DOE/EERE, DOD, industry, the Small Business Innovation Research program, and the Small Business Vouchers Pilot program.

8. Climate change sciences and atmospheric science

*Capability*

Argonne’s strengths in climate change and atmospheric sciences have historically rested in our ability to make sophisticated atmospheric measurements at large scale and under unique circumstances (for example, on board an ocean-going ship) and to do advanced climate change simulations in high-performance computing environments. We also have maintained a strong focus on soil science, which has evolved to include geospatial analytics to extend field measurements and understanding. We have pioneered the application of synchrotron technology to perform chemical and physical analyses of atmospheric dust and aerosols as well as soils.

Our strategy under this capability is to weave together the following objectives and leverage their synergies to provide outstanding science:

- Operate the ARM-SGP site as an outstanding facility through expert management and responsiveness to facility users and continually grow our deep understanding of sensor technology and enhance the facility’s measurement capabilities
- Use Argonne’s renowned expertise in applied mathematics, computer science, and high-performance computing to promote the software and computational objectives of DOE/SC-BER’s Accelerated Climate Modeling for Energy (ACME) project and to support the data and analytic needs of other DOE R&D areas related to climate and atmospheric science, such as energy-water interdependence
- Enrich our aerosol/cloud science expertise to complement our ARM facility strengths and expand the use of ARM data in our climate research, including a collaboration with Brookhaven National Laboratory in cloud and aerosol research under a DOE/SC-BER science focus area
- Integrate our atmospheric and hydrologic expertise to develop predictive capabilities relevant to understanding infrastructure vulnerability to adverse weather and flooding under climate change
- Focus our soil and geospatial analytics expertise on reducing uncertainty in estimates of global soil carbon stocks and their vulnerability to climate change, especially in the Arctic

The ARM-SGP facility supports studies of the effects of aerosols, precipitation, surface flux, and clouds at global, regional, and local climate and weather scales. We recently enhanced our ARM-SGP soil moisture measurements and, through discretionary investments, we are developing hyperspectral sensor technology to continuously characterize vegetation, as well as technology to enable multisensor intelligent networks for climate measurements, and we are gaining experience in aerial unmanned systems for atmospheric measurements. Our ARM-SGP mentors are working with other research organizations to incorporate ARM measurement analyses into several science campaigns, such as the recent ARM West Antarctic Radiation Experiment (AWARE) campaign.

Our staff of atmospheric scientists with aerosol and cloud science expertise have identified the importance of light-absorbing organic carbon in the earth’s radiation budget and, through the use of the APS, determined the chemical changes that aerosols undergo as they cross the Atlantic. This staff now
anchors our contribution to a collaboration with BNL in cloud and aerosol research under a DOE/SC-BER science focus area as well as our incorporation of land cover change, aerosol, and dust science into ACME. Eleven Argonne scientists apply ALCF capabilities in support of DOE/SC-BER earth systems modeling and atmospheric sciences: with Strategic Partnership Project support, we have used the ALCF to simulate the North American climate for 1980-2090 at the most detailed resolution (12 km) ever achieved. We are leveraging this effort to simulate future weather and hydrology at a regional scale to predict infrastructure vulnerability.

Mission relevance and funding

This core capability supports the missions of DOE/SC-BER and other federal entities with climate and atmospheric science initiatives. Current additional sponsors include DOD, DOI, and EPA.

9. Computational science

Capability

Computational science, a cornerstone of Argonne’s R&D enterprise, advances critical problems in many scientific disciplines. Our Laboratory-wide computational activities include more than 350 scientists and engineers, working in interdisciplinary project teams with embedded applied mathematicians and computer scientists. Argonne’s computational science capability includes and leverages the hardware and expertise within ALCF, our Joint Laboratory for System Evaluation, and our Laboratory Computing Resource Center.

We will continue to enhance and promote our computational science capabilities across the Laboratory, and to the scientific community at large, in the following ways:

- Tightly integrate ALCF and APS capabilities for large-scale data analysis and machine-in-the-loop experiments by creating a center for fluid modeling development that targets a wide range of applications, expands and coordinates our computational materials science capabilities, and serves as a data hub for large-scale data curation and analysis that will help drive our development of machine learning in science
- Develop new statistical frameworks that reduce modeling complexity and automatically identify and configure the best machine learning algorithms to meet the required objectives for a given problem
- Place and co-mentor computational postdoctoral appointees across Argonne and appoint data science points of contact (POCs) in each directorate (computational science POCs are already in place)
- Make ALCF staff available to guide computational science groups as they apply for DOE’s Innovative and Novel Computational Impact on Theory and Experiment and ASCR Leadership Computing Challenge awards, and make ALCF resources available through Director’s Discretionary awards

Examples of the impact and leadership of Argonne’s computational science capability include:

- One of the world’s largest high-resolution cosmological simulations, modeling the universe over billions of years, and algorithms and toolkits for analysis of large datasets from APS and the Large Hadron Collider (LHC) in Switzerland, where ALCF’s Mira supercomputer was the seventh largest provider of cycles to the LHC’s ATLAS experiment and where ALCF improved ALPGEN, a key component of the LHC-ATLAS workload, to run 23 times faster
- Innovative modeling of nuclear reactors (Nek5000, UNIC, OpenMC)
- Development of and contributions to additional applications: elegant (accelerator simulation), TomoPy (x-ray tomographic analysis), and Green’s Function Monte Carlo (properties of nuclei; revealed new details of the carbon-12 nucleus structure and is enabling research that will improve understanding of subatomic particles)

- Collaborative projects that have benefited industry and academia, such as Argonne’s Virtual Engine Research Institute and Fuels Initiative, in which simulations have revealed key insights into fuel injection timing in internal combustion engines, and the Joint Center for Energy Storage Research, for which a key simulation code written for a conventional computer was modified to run 30 times faster on Mira

**Mission relevance and funding**

This core capability supports missions across all of DOE and other entities that fund research and development. Current sponsors include ARPA-E; DOE/EERE; DOE/OE; DOE/SC-ASCR, -BER, -BES, -FES, -HEP, and -NP; NIH; NSF; and industry.

10. **Condensed matter physics and materials science**

   **Capability**

   Argonne’s internationally recognized research elucidates fundamental properties of materials and uses this knowledge to create materials with a desired functionality that can be translated for potential applications. Our leadership is grounded in the integration of the APS, CNM, and ALCF with diverse expertise in materials and chemistry. Our approach is reflected in Argonne’s strategic plan for materials research, which emphasizes defects and interfaces as an overarching theme that is exploited in the focus areas of quantum and spin coherent matter, soft matter and hybrid materials, and electrochemical phenomena and clusters. Materials of emphasis include superconducting, magnetic, and catalytic materials; quantum metamaterials; ferroelectrics; correlated oxides; and, more recently, topological materials and electrochemical oxides.

   Argonne’s suite of capabilities include single crystal growth, greatly enabled by our unique high-pressure floating zone furnace; molecular beam epitaxy (MBE), highlighted by our new 4D/5D oxide MBE; and thin film growth. This suite is being enhanced by the installation of a unique aluminum nitride deposition system in our Materials for Energy Module (MEM) and by internal discretionary investments in an Argonne “quantum factory” that will specialize in the growth of oxide, nitride, and chalcogenide thin films. Our capabilities in materials characterization include coherent diffraction, which allows us to image the strain fields around individual defects; full 3D diffuse x-ray and neutron scattering; terahertz dynamics; and our Lorentz microscope for imaging vector magnetization. We also conduct leading research in vortex physics, spintronics, and electrochemistry, with an emphasis on *in situ* studies coupled to modeling and simulation.

   Several key collaborations complement these capabilities: (1) the UChicago-Argonne Institute for Molecular Engineering (IME), which focuses on computational materials science, polymeric and bio-inspired materials, and quantum engineering; (2) the Midwest Integrated Center for Computational Materials (MICCoM), funded by DOE/SC-BES to develop and disseminate computational tools to simulate and predict properties of functional materials for energy conversion processes; (3) two DOE/SC-BES Energy Frontier Research Centers – the Argonne-Northwestern Solar Energy Research Center and the Center for Emergent Superconductivity; and (4) two synergistic centers in energy storage funded by DOE/SC-BES – the Center for Electrochemical Energy Science and the Joint Center for Energy Storage Research (JCESR), an Energy Innovation Hub.

   JCESR, which Argonne leads, has advanced its three legacies in fundamental science, transformative research prototypes for transportation and grid batteries, and a new paradigm for battery R&D that integrates discovery science, battery design, research prototypes, and manufacturing collaboration.
JCESR’s science legacy is well established, with significant advances in broad energy storage science and in science for specific prototypes, and its new paradigm is fully operational. While challenges remain to deliver pre-commercial prototypes, we are on track to achieve this goal as well.

Argonne’s condensed matter physics and materials science research is strongly coupled with simulation capabilities at the ALCF and unique experimental tools at the APS and CNM, along with those of other DOE/SC-BES facilities, principally the SNS and LCLS. Looking to the future, the planned APS and ALCF upgrades will provide critical new abilities to accelerate our materials breakthroughs. In addition, the Materials Design Laboratory being built at Argonne will provide state-of-the-art capabilities and interdisciplinary synergies that extend those already realized with the adjacent MEM and Energy Sciences Building. Our management strategy for IME and MICoM emphasizes maximizing their benefit to both Argonne and DOE, and investments of discretionary resources have allowed us to seed new research directions to evolve our programs.

Mission relevance and funding

This core capability supports the missions of DOE/SC-BES and other DOE/SC programs. Additional sponsors include DOE/EERE, DOD, and industry.

11. Cyber and information sciences

Capability overview

Our core capability in cyber and information sciences is one of three – in synergy with our decision science and analysis capability and our systems engineering and integration capability – that position Argonne to deliver effective solutions to complex, multidisciplinary problems. We leverage these three capabilities to enable the science basis for a national and global infrastructure that is more resilient, enables increased energy efficiency, enhances mobility and quality of life, and strengthens national and homeland security.

For more than 40 years, Argonne has advanced modeling and experimental R&D in the areas of information sciences, decision-making, and integrated system development for DOE, DHS, other federal agencies, and industry. Application areas include cybersecurity, national security and intelligence analyses, critical infrastructure assessment, and transportation modeling. This research significantly leverages the ALCF, including petascale computing, and the APS experimental capabilities, and draws on Argonne’s materials, chemistry, and engineering capabilities.

Our breadth of expertise in this area positions us to support decisions regarding emerging topics of national importance, such as electric grid design and reliability, energy-water interdependence, urbanization, the Internet of Things, and automated vehicles. We explore these widely scoped problems in partnerships with researchers in universities, at other national laboratories, and in the private sector, to deliver results that have global impact. Argonne’s ability to bring multidisciplinary teams together is key to our long-standing recognition in this area.

In cyber and information sciences, we help protect the nation as a key, trusted partner to federal and state government agencies, through our research into the resiliency of critical cyber assets, the security of cyber-physical systems, and the collection and dissemination of intelligence needed to defend against cyber threats. More than 50 staff members are dedicated to the cybersecurity mission in a wide range of areas, including:

- Cybersecurity research in data analysis, energy resiliency, intelligent log analysis, authentication, infrastructure risk assessment, moving target defense, vehicle security, power grid cyber susceptibility, and technologies to increase resilience and improve national security
- Sharing of cyber threat information using real-time, machine-to-machine methods in support of the DOE enterprise, the energy sector, and other federal entities using the Cyber Fed Model
system, which Argonne runs as DOE’s primary system for sharing cyber threat information and which supports DOE’s roles as the Sector Specific Agency for the energy sector and in the Cybersecurity Information Sharing Act of 2015

- Design of tools for evaluating the resiliency, interdependency, and defenses of computer systems that operate critical infrastructure, as well as the consequences of attacks on those systems
- Creation of regional cyber resiliency plans
- Development of techniques for offensive cybersecurity programs
- Conduct of both quick-turnaround and long-term assessments of cyber threats, vulnerabilities, consequences, and dependencies

Facilities that support this core capability include enterprise data centers that host a multi-agency secure private cloud and state-of-the-art facilities for analyzing the cyber security of vehicles.

Mission relevance and funding

This capability, in concert with our capabilities in decision science and analysis and in systems engineering and integration, supports the missions of DOE, DHS, other federal agencies, and industry. Current sponsors include DOE/EERE, DOE/EPSSA, DOE/IN, DOE/NE, DOE/NNSA, DOE/OCIO, DOE/OE, DOD, DOS, DOT, NERC, NGA, NIH, NSA, and NSF. Argonne’s DHS sponsors include CS&C, FEMA, FPS, I&A, IP, OCIA, PSCD, and TSA.

12. Decision science and analysis

Capability overview

Our core capability in decision science and analysis is one of three – in synergy with our cyber and information science capability and our systems engineering and integration capability – that position Argonne to deliver effective solutions to complex, multidisciplinary problems. We leverage these three capabilities to enable the science basis for a national and global infrastructure that is more resilient, enables increased energy efficiency, enhances mobility and quality of life, and strengthens national and homeland security.

We view these three capabilities as a fully integrated set of competencies that we apply to solving some of the most complex problems our country faces. Argonne’s experience in and approach to this work are discussed in more detail in the description of our cyber and information science capability.

In decision science and analysis, Argonne combines rich expertise in systems and decision analysis with computer simulation to apply science to inform government decision-making. With more than 200 staff members working in decision science and analysis, we are recognized for addressing pressing national challenges through innovative applications of agent-based modeling, complex adaptive system modeling, system dynamics, complex network analysis, and life-cycle analysis. Argonne approaches problems not in isolation, but as dynamic and interrelated systems. We combine this approach with traditional deterministic methods to better inform decision makers on ways to address the complex problems of today.

Facilities that support this work include an immersive decision visualization studio and the ALCF; leadership computing has notably been applied to the analysis of social and behavioral systems, including predictive modeling of the spread of infectious disease in urban areas and the mitigating effects of interventions.

We have provided national and international leadership in the application of novel agent-based modeling approaches, development of bottom-up approaches to understanding supply chains and market, evaluation of alternatives for interdependencies, recovery and resilience of lifeline
infrastructures with a particular focus on the electric grid, analysis of social dynamics applied to energy and national security issues, and analysis of the energy and environmental impacts of vehicle and fuel technologies. We are extending our decision science capabilities beyond traditional energy infrastructure assessments to address emerging problems in energy-water interdependence and urban sciences. As we move our capability forward, we expect to make increasing usage of advanced computing approaches and architectures, including exascale and machine learning.

Mission relevance and funding

This capability, in concert with our capabilities in cyber and information science and in systems engineering and integration, supports the missions of DOE, DHS, other federal agencies, and industry. Current sponsors include DOE/EERE, DOE/EPSA, DOE/IN, DOE/NE, DOE/NNSA, DOE/OCIO, DOE/OE, DOD, DOS, DOT, NERC, NGA, NIH, NSA, and NSF. Argonne’s DHS sponsors include CS&C, FEMA, FPS, I&A, IP, OCIA, PSCD, and TSA.

13. Large-scale user facilities / advanced instrumentation

Capability

Argonne is a leader in the design, construction, and operation of world-class scientific user facilities. Our four on-site facilities – ALCF, APS, ATLAS, and CNM – together served 7400+ users in FY16, one of the largest user communities in the DOE system. In addition, for DOE/SC-BER, we operate the ARM-SGP site, which supplied data to 500+ users in FY16. Effective management of large facility-user programs and synergistic, cross-disciplinary collaboration across facilities are key elements of our overarching mission for DOE. The APS and ATLAS also contribute to and draw heavily on our core capability in accelerator science and technology.

ALCF, funded by DOE/SC-ASCR, operates an IBM Blue Gene/Q system (Mira), one of the world’s largest supercomputers dedicated to open science; deployed a Cray XC class system (Theta) in late 2016 that will transition to production in 2017; and will deploy an Intel system (Aurora) in 2021. The ALCF provides petascale-computing capabilities that enable the computational science and engineering community to run the largest and most complex applications. It also hosts the Joint Laboratory for System Evaluation, which gives our staff and collaborators access to the latest production and prototype computing resources.

APS is a DOE/SC-BES facility with additional investments by other DOE offices including SC-BER and NNSA, EPA, NIH, NSF, universities, and industry. It is an internationally leading source of high-energy x-rays enabled by Argonne’s expertise in x-ray science, instrumentation, insertion devices, optics, and accelerator physics. Capabilities include high-energy scattering; in situ investigation in high-pressure, high-magnetic-field, synthesis, and other environments; operando studies; imaging and spectroscopy experiments; macromolecular crystallography; studies of shock physics; and x-ray interrogation of electron and lattice excitations. We are planning the APS Upgrade project, to increase x-ray brightness and coherent flux by two to three orders of magnitude; our plans include measures to prepare current APS users to take full advantage of the upgrade and minimize impact on their work during the one-year APS shutdown expected during the upgrade.

CNM, funded by DOE/SC-BES, provides expertise, instruments, and infrastructure for interdisciplinary nanoscience and nanotechnology research. Its unique capabilities include near-field optical measurements at the extremes of space and time resolution from the ultraviolet to the terahertz as well as broad capabilities in scanning tunneling microscopy and cleanroom-based nanofabrication. Looking forward, CNM’s strategy for serving the user community emphasizes quantum materials; manipulating nanoscale interactions; synthesis of nano-architectures for energy, information, and functionality; and a new focus on combining data science with electron microscopy. Collaborative efforts with APS include upgrade planning for the jointly operated hard x-ray nanoprobe and partnerships on the synchrotron x-
ray scanning tunneling microscope and on nanofocusing and beam-deflecting x-ray optics. Ongoing multimodal imaging efforts leverage both APS and CNM.

ARM-SGP, funded by DOE/SC-BER, is the world's largest and most extensive climate research field site. Its instruments are arrayed across 9,000 square miles, with a heavily instrumented central facility on 160 acres near Lamont, Oklahoma. Scientists from Argonne and other institutions use data from ARM-SGP to learn about cloud, aerosol, and atmospheric processes, which supports improvements in models of the earth's climate.

ATLAS, funded by DOE/SC-NP, is a superconducting linear accelerator and the only DOE user facility for low-energy nuclear research. It provides high-intensity heavy-ion beams in the energy domain best suited to study the properties of the nucleus. At ATLAS, the CARIBU facility has the unique capability to provide both stopped and reaccelerated beams of radioactive neutron-rich nuclei. ATLAS offers its users an array of unique experimental systems to take full advantage of the accelerator capabilities.

Mission relevance and funding

This core capability supports the DOE-SC mission to operate scientific user facilities that provide the highly advanced research tools needed to address the world's greatest challenges in science and technology. Our facilities are sponsored by DOE/SC-ASCR, -BER, -BES, and -NP; support for specific experiments also is provided DOE/NNSA, DOE/OE, NIH, NSF, and industry.

14. Nuclear and radio chemistry

Capability

Argonne has executed pioneering work in chemical separations, nuclear chemical engineering, and the materials and chemical science of actinides, radioisotopes, and the nuclear fuel cycle. Our strategy to maintain and build on this capability includes gaining new understanding of the:

- Structure-property relationships behind actinide chemistry and solvent extraction across a broad spectrum of energy-related areas, from nuclear fuel and material separations to radioisotope production
- Critical ion-ion correlations that underpin effective syntheses of transuranic materials and drive actinide/fission-product separations
- Technical basis for next-generation separations and safeguards technologies for future nuclear energy systems

We leverage a distinctive portfolio of research capabilities and facilities that enable this work, including:

- APS, ATLAS, and ALCF
- Electron microscopy tools
- Two co-located, purpose-built radiological facilities: a low-energy electron linear accelerator and a chemical separations system for radioisotope production and isolation
- Radiological laboratories that enable us to develop and test advanced electrochemical and aqueous processes, to support development of innovative nuclear fuel cycle and safeguard technologies

These capabilities are applied to actinide science that pioneers novel approaches to the synthesis, characterization, and modeling of transuranic complexes. Purpose-built radiological facilities are used to extend understanding of the chemistry of these man-made elements. Predictive bonding and energetics models are targeted, within the context of separations relevant to nuclear energy, by using Argonne computational facilities to interpret x-ray data made available through the APS. We are developing capabilities in accelerator-based radioisotope production for medical and research applications, with
associated separation and purification technologies. We also conduct sensor and detector research for
national programs in border, cargo, and transportation security, as well as chemical, biological,
radiological, and nuclear incident mitigation; our focus includes millimeter wave technologies for
remote detection and sensors, as well as forensics to identify sources of nuclear and biological
materials.

Mission relevance and funding

This core capability supports the missions of DOE and other organizations that seek to advance
understanding of actinide chemistry, radioisotopes, and technologies for future nuclear energy systems.
Current sponsors include DOE/NE, DOE/NNSA, DOE/SC-BES and -NP, and overseas organizations.

15. Nuclear engineering

Capability

Argonne pioneered nuclear energy systems and continues to be a world leader in advancing nuclear
science and technology. We are recognized for groundbreaking research in both advanced nuclear
energy technology and nuclear materials security. Our nuclear engineering capability broadly supports
nuclear energy development, nuclear nonproliferation, nuclear physics in areas of isotope research and
production, nuclear instrumentation, and protection of critical infrastructure. More than 300 staff
members support our nuclear capability. Throughout our history, we have emphasized national and
international collaboration with research and industrial partners.

Argonne’s nuclear engineering strategy has five major components:

- Establishing the science basis for verifying safety, sustainability, and regulation of existing nuclear
  systems
- Leading, in partnership with Idaho National Laboratory (INL) and Oak Ridge National Laboratory
  (ORNL), innovation for next-generation nuclear technologies, including reactor and fuel cycle
design
- Leading, in partnership with INL and ORNL, the development of the future R&D infrastructure for
  nuclear technology, including a new fast test reactor
- Leading the development of the science and technology basis for nuclear nonproliferation,
  including minimizing the use and availability of highly enriched uranium
- Advancing the DOE/SC-NP goals for isotope production and research.

We have applied our understanding of reactor physics to the design of nuclear systems and fuel
cycles and to the conversion of fuel in research and test reactors around the world from highly enriched
to low-enriched uranium. We have demonstrated our fuel conversion leadership through technical
analyses and assessments that support a number of federal agencies, including the assessment of the
redesigned Iranian Arak heavy-water reactor in support of the 2015 Joint Comprehensive Plan of Action
agreed upon by the United States, Iran and other nations.

Argonne is viewed as the world leader in designing and analyzing fast neutron spectrum systems,
contributing to resolution of nuclear safety issues, and understanding the performance of fuels and
materials in nuclear reactors. Our understanding of severe nuclear accident behavior is widely
recognized by the international community, and we have been a leader in understanding actinide
chemistry and various techniques for separating radioisotopes.

Nuclear engineering R&D leverages Argonne’s strengths in materials science, nuclear and radio
chemistry, nuclear physics, X-ray imaging, and computational science. Key facilities that support this
work include APS; ALCF; ATLAS; and our Intermediate Voltage Electron Microscopy-Tandem Facility,
which has unique capabilities to image changes in materials during irradiation. This work is also supported by our specialized engineering development laboratories for detailed studies of reactor components and separations flowsheets under prototypic conditions through the engineering scale. Using ALCF, Argonne has made groundbreaking advances in exploiting high-performance computing for multiphysics analysis of nuclear-reactor behavior.

**Mission relevance and funding**

This core capability supports the missions of DOE and other organizations to sustain the benefits of nuclear energy generation, develop new and innovative nuclear energy systems, and enhance the security of nuclear technology applications worldwide. Current sponsors include DOE/NE, DOE/NNSA, DOE/SC-NP, DHS, NRC, the nuclear power industry, and international organizations.

16. Nuclear physics

**Capability**

Argonne’s theoretical and experimental nuclear physics research provides globally recognized leadership in nuclear structure, nuclear astrophysics, fundamental interactions, medium energy physics, and, more broadly, in nuclear instrumentation, accelerator development, and selected applications. Key to our work is ATLAS, which provides stable and radioactive ion beams at energies up to about 20 megarayons/nucleon. Argonne staff and visiting scientists use ATLAS to highlight aspects of nuclear structure that vary strongly with the proton-to-neutron ratio and are not readily apparent in stable nuclei, to investigate reactions and nuclear properties far from stability as the basis of astrophysical processes generating the chemical elements, and to test nature’s fundamental symmetries and interactions.

Our physicists are leaders in studying the underlying strong force and its foundation in quantum chromodynamics as it applies to protons and neutrons and to the strongly coupled nuclear many-body system. They design, construct, and operate detectors at Thomas Jefferson National Accelerator Facility (TJNAF) and Fermilab to carry out these investigations. Argonne staff members lead the SeaQuest experiment at Fermilab, including a search for dark photons, and are principal investigators for about 30% of all approved experiments in TJNAF’s 12-gigaelectron-volt program. At Argonne, we search for violation of time reversal symmetry using an electric dipole moment measurement of radium-225 as a probe for physics beyond the Standard Model. Argonne’s nuclear and particle physicists collaborate to perform simulations, accelerator R&D, and detector R&D for electron-ion collider concepts.

Argonne’s experimental programs in nuclear physics are supported by our work in accelerator science and technology and by widely recognized theory efforts that leverage the ALCF and our computer science capabilities. We are leaders in quantum Monte Carlo calculations of nuclear structure and reactions, and predictions of hadron and nuclear properties using nonperturbative methods in continuum quantum chromodynamics. Applications include characterization of spent nuclear fuel for reactor design; production techniques for medical radioisotopes; and radio-krypton and radio-argon dating with atom traps for geophysical, oceanography, and fundamental research. We have begun construction of a national center for radio-krypton dating, with the capability to expand to include radio-argon dating.

Multiple upgrades have kept ATLAS at the forefront of discovery, providing capabilities that include:

- Superconducting radio-frequency structures with cutting-edge performance, providing total accelerating voltages in excess of 55 megavolts
- High-purity ion beams of radioactive isotopes not available anywhere else in the world, from the Californium Rare Ion Breeder Upgrade (CARIBU) to ATLAS
• State-of-the-art instrumentation such as Gammasphere (the national gamma-ray facility), HELIOS (a helical orbit spectrometer), the Canadian Penning Trap mass spectrometer, ion and atom traps, and a fragment mass analyzer

Further upgrades to ATLAS are underway, including a gas-filled separator, an in-flight radioactive ion separator, and projects to more than double the intensity of re-accelerated CARIBU beams using an electron-beam ion source charge breeder and to deliver stable heavy ions with tens of particle microampere intensities. To address high demand from the user community for ATLAS beam time, a concept for a multi-user capability is being developed where two beams of different species and energies would be delivered at the same time to separate experimental areas.

Mission relevance and funding

This core capability supports the DOE/SC-NP mission. Additional current sponsors include DOE/SC-BES and -HEP; IAEA; NSF; and universities in the United States and abroad.

17. Particle physics

 Capability

Argonne’s particle physics research advances the understanding of the properties and interactions of the energy-matter composition of the universe and the underlying symmetries of nature. This work, with a track record of many significant contributions and leadership roles, distinguishes itself through the strong synergies and collaborative efforts across the Laboratory and the DOE complex in collaboration with UChicago and Northwestern University.

Our research in theoretical and computational cosmology provides the most accurate, large-volume, dynamic evolution of the universe that is currently available. Our High Energy Physics Division closely collaborates with our Mathematics and Computer Science Division, the ALCF, and other DOE laboratories, and plays a leadership role in extracting science from current and future cosmological surveys. By developing the Hybrid/Hardware Accelerated Cosmology Code framework and the data analysis library CosmoTools, Argonne has become a leader in extreme-scale, high-resolution cosmological simulations. Run at the ALCF and other DOE leadership computing facilities, these computational tools generate synthetic sky maps that enable current construction projects to exercise their data analysis pipelines and provide comparisons with actual observations to give, for example, insights into the dark sector of the universe. We aim to provide advanced statistical community tools to extract science from the next-generation DOE and NASA surveys. Our cosmology group also leads one of the exascale computing project funded by DOE/SC-ASCR.

Through collaborative, multidisciplinary efforts across Argonne, we have successfully pioneered the development of novel detectors, such as large-area photo-detectors with picosecond timing resolution and wafer-scale multichroic transition edge sensors for cosmic microwave background measurements. To leverage Laboratory-wide synergies in future sensor and detector development, we are establishing formal coordination mechanisms that will support multiple initiatives.

To strengthen the overall program at the Large Hadron Collider (LHC) in Switzerland, we are transitioning our focus away from calorimetry to the construction of a new pixel detector, development of state-of-the-art trigger hardware and software, and creation of meta-databases and new input/output frameworks. Through the high energy physics community’s Center for Computational Excellence, co-led by Argonne, high-performance computing tools are being developed to ultimately use the power of exascale architectures and systems for high energy physics. First-of-a-kind simulations of LHC particle collisions that were carried out using the ALCF have enabled publication of results from the LHC’s ATLAS experiment that would otherwise not have been possible. Our particle theory research, using the ALCF, has provided the most precise theoretical quantum chromodynamics predictions for
standard model processes, essential to search for new physics, a research area in which Argonne has been active.

We lead the testing and calibration of the magnetic field map for the g-2 and Mu2e experiments being built at Fermilab, and have taken on critical roles in the construction of liquid-argon-based neutrino detectors. (The Argonne Wakefield Accelerator is described under the accelerator science and technology core capability.)

**Mission relevance and funding**

This core capability supports the DOE/SC-HEP mission and is well aligned with the national high energy physics roadmap. Additional current sponsors include DOE/SC-ASCR and -BES as well as NASA.

18. **Systems engineering and integration**

**Capability**

Our core capability in systems engineering and integration is one of three – in synergy with our cyber and information science capability and our decision science and analysis capability – that position Argonne to deliver effective solutions to complex, multidisciplinary problems. We leverage these three capabilities to enable the science basis for a national and global infrastructure that is more resilient, enables increased energy efficiency, enhances mobility and quality of life, and strengthens national and homeland security.

We view these three capabilities as a fully integrated set of competencies that we apply to solving some of the most complex problems our country faces. Argonne’s experience in and approach to this work are described in more detail in the description of our cyber and information science capability.

In systems engineering and integration, our capstone R&D programs are supported by crosscutting systems capabilities that strongly leverage basic research and major scientific user facilities. We are recognized for developing experimental facilities and analytical tools to advance understanding of infrastructure, urban, communications, and other large-scale systems, and we apply our transportation systems engineering capabilities to identify efficiencies that reduce pollutants. Argonne facilities used in this work include:

- The APS, used to study fuel injector spray dynamics and combustion chemistry in automotive engines; Advanced Powertrain Research Facility, used to evaluate vehicle propulsion systems; and Engine Research Facility, used to study in-cylinder combustion, fuels, and emissions under operating conditions
- Tribological benchtop laboratories, used to define, evaluate, and improve material coatings, lubricant additives, and thermal efficiency for product longevity, friction reduction, and energy efficiency
- Electric Vehicle – Smart Grid Interoperability Center, with sister facilities overseas operated by the European Commission, used to conduct research to facilitate transatlantic interoperability between electric vehicles and their charging infrastructure, ultimately leading to smart-grid integration

Our expertise in vehicle energy consumption is leveraged for U.S. manufacturing job retention through our ongoing collaborations with the European Commission, industrial partners, and the U.S.-China Clean Energy Research Center’s Clean Vehicles Consortium.

Argonne is nationally recognized for developing methods to help solve security, risk, resiliency, and interdependency problems facing lifeline infrastructures. In complementary work, the joint Argonne-UChicago Urban Center for Computation and Data provides resources and tools to address the global challenges created by rapid urbanization and aging cities. Additionally, as part of the DOE Grid
Modernization Laboratory Consortium and in partnership with industry, we are developing analytical and modeling tools, including advanced computational algorithms, to drive improvements in our nation’s electrical infrastructure.

**Mission relevance and funding**

This capability, in concert with our capabilities in cyber and information science and in decision science and analysis, supports the missions of DOE, DHS, other federal agencies, and industry. Current sponsors include DOE/EEERE, DOE/EPSA, DOE/IN, DOE/NE, DOE/NNSA, DOE/OCIO, DOE/OE, DOD, DOS, DOT, NERC, NGA, NIH, NSA, and NSF. Argonne’s DHS sponsors include CS&C, FEMA, FPS, I&A, IP, OCIA, PSCD, and TSA.

**Science Strategy for the Future**

Through Argonne’s major initiatives, we are committed to significantly expanding our contributions to fundamental knowledge and to the foundations for technologies that will shape our nation’s future. Because we are a nexus for more than 8000 facility users and collaborators annually, our innovations through these initiatives will have broad impact beyond Argonne. Our major initiatives for the next five to ten years are interdisciplinary and highly synergistic with one another and with our broader research and development (R&D) enterprise. They are intended to deliver breakthroughs in science and technology in five areas that support DOE’s missions and reflect our vision for our future:

- Hard x-ray sciences
- Advanced computing
- Materials and chemistry
- The universe as our laboratory
- Energy manufacturing science and engineering

Our initiatives build on our distinguishing capabilities in science, facilities, and external collaboration networks. Those capabilities start with our science and engineering expertise in chemistry, materials, physics, and accelerators, and our leadership in applied mathematics and computing sciences. That expertise is complemented by our unmatched suite of co-located major facilities: the Advanced Photon Source (APS), Argonne Leadership Computing Facility (ALCF), Center for Nanoscale Materials (CNM), and Argonne Tandem Linear Accelerator System (ATLAS). Our robust network of collaboration provides a third foundation for our initiatives, starting with the University of Chicago (UChicago) and extending to other leading research universities, other research laboratories, and American industry.

**Infrastructure**

**Overview of Site Facilities and Infrastructure**

Argonne National Laboratory is located on 1,517 acres about 25 miles southwest of Chicago, in DuPage County, Illinois. The site includes 157 buildings totaling 4,970,903 gross square feet (SF). Argonne’s site, overseen by DOE/SC, accommodates about 12,800 persons yearly, including Argonne and DOE employees, contractors, facility users, visiting scientists, and students.

In addition to buildings operated by Argonne, the site includes the Howard T. Ricketts Regional Biocontainment Laboratory, operated by the University of Chicago; and the Theory and Computing Sciences Building, a privately operated building in which Argonne leases about 240,000 SF. Building 350, formerly operated by DOE as the New Brunswick Laboratory, was transferred to Argonne in FY17.

The average age of the Argonne-operated facilities and infrastructure is 48 years, with more than 60% of the assets being more than 50 years old. Our facilities are roughly 90% occupied. The condition
of these facilities by gross square footage, as defined by the DOE Laboratory Operations Board’s criteria, is 35% adequate, 64% substandard, and 1% inadequate. For mission-critical facilities, the site’s asset condition index (ACI) is 0.98 (excellent). The ACI is based on identified deferred maintenance as it relates to the estimated plant replacement value. The average ACI for all facilities and infrastructure is 0.94 (adequate).

No real estate actions – including new (or renewal) leases of 10,000 SF or more or disposals of DOE land via leasing, sale, or gift – were executed in FY16. For FY17, a 10,000 SF lease to SBA Towers, LLC, is currently planned to support a multiprovider cellular tower, which will significantly improve cellular service on the Argonne site and in neighboring communities.

Campus Strategy

Overview

We have developed a structured, 10-year site modernization plan – entitled Facility and Infrastructure Strategic Investment Plan – to revitalize and construct facilities and infrastructure to meet current and emerging mission needs. The plan addresses environmental performance, safety, legacy waste, obsolete facilities, new facilities, and operating and maintenance support. Needs identified in the plan are prioritized, with timing and sequencing of actions chosen to align with the mission and leverage resources available for execution. The locations of proposed investments are summarized in Figure 6.1, with the details of the investment plan presented in Tables 6.1 and 6.2.

Four main principles guide our campus strategy:

- **Support mission-critical programs.** Argonne continues to commit internal resources and communicate needs for external funding to establish an executable plan for supporting immediate and future infrastructure investments required for mission-critical programs.

- **Construct replacement facilities and re-use/renovate existing facilities.** We renovate and modernize existing facilities to meet current and future scientific laboratory facility needs while reducing deferred maintenance and increasing utilization rates. These efforts apply overhead investment to enable re-use of facilities that, although obsolete due to age, retain positive structural and space characteristics that support modern scientific research.

- **Address support infrastructure.** Argonne continues to maintain a rigorous process for assessing building and site infrastructure conditions to prioritize and implement repairs and upgrades to meet reliability and redundancy goals. We are committed to reducing our identified deferred maintenance backlog, with an ultimate target of achieving the DOE-established goal for “adequate” condition for all facilities and infrastructure.
Figure 6.1 Locations of proposed investments under ten-year campus infrastructure strategy

- **Address legacy waste and excess facilities.** Removal of legacy waste and excess facilities is consistent with the DOE/SC goal of achieving an asset utilization index ratio of 1:1. It also supports complex-wide DOE requirements for overall footprint reductions via space banking. As of April 2016, Argonne’s estimated unfunded, nonrecurring liability totaled $591 million, based on recent in-house evaluations of the remaining legacy facilities. We are aggressively consolidating radiological facilities and reducing inventories of radiological materials, while preserving the capability to perform mission-important activities. Partnering with DOE to identify stable funding is required for expeditious cleanup, material and waste disposition, and ultimate disposition of these facilities. Argonne has requested DOE/EM funding to remove several contaminated facilities that are or will become inactive in FY17 - FY28; however, due to federal budget constraints, there is a high probability we will not receive funding within the proposed timeframe.

**Key investments**

**Materials Design Laboratory ($95M SLI)**

The Materials Design Laboratory (MDL) is currently under construction and on schedule for completion within cost, scope, and schedule. This 115,000 SF facility will enable continued consolidation of research space that began with the Energy Sciences Building (ESB), to support three closely associated core capabilities: condensed matter physics and materials science, chemical and molecular science, and chemical engineering. This high-performance laboratory building will include high-accuracy, flexible, and sustainable space needed to support scientific theory/simulation, materials discovery, characterization, and application of new energy-related materials and processes.
Argonne redundant power supply ($60M SLI)

An upgrade to Argonne’s high-voltage power supply is required to support projected load increases associated with scientific growth and to provide a fully redundant power supply to all site research programs, facilities, and systems. Argonne today receives power from a single location that, along with the associated 549A main substation yard, have original 1960 equipment and installations. This condition increases the risk of an external power outage impacting the site and mission-critical programs, including APS, CNM, ALCF, and ATLAS. The power upgrade also will provide additional capacity to support increases in electrical usage associated with exascale computing efforts estimated in the 2021-2022 timeframe. Complementary site electrical redundancy improvements are proposed with IGPP funding to address additional aging facility issues that may reduce site electrical distribution reliability.

Building 375 high bay reutilization ($6.3M GPP)

We have identified the high bay in Building 375 as one of the locations on site that can support the APS Upgrade project’s space needs for preparatory activities before the planned 2022-2023 shutdown of APS for the upgrade. This high bay, which can provide about 11,250 SF of crane-covered space adjacent to existing APS operations, is currently not used due to contamination associated with an abandoned monolith in that space, which was part of the former Intense Pulsed Neutron Source program. Once the monolith is removed, this building’s utilization will increase from 44% to 100% and eliminate legacy waste from Argonne’s portfolio.

Underground utility modernization ($8.5M GPP)

Much of Argonne’s underground piping distribution for water and sewer is original to the site and in substandard or inadequate condition. In FY17, we initiated an intensive planning effort to prioritize critical locations for replacement of piping over a multiyear, phased modernization program. Direct funding is required to address about 43,430 feet of underground water and sewer piping while internal IGPP investments are proposed to upgrade the distribution and capacity associated with the site’s chilled water system. Additional internal maintenance and repair funding will address deficiencies at our wastewater treatment facility, which currently experiences overflow conditions that pose operational and environmental risk to the site and surrounding areas during heavy rain events.

APS area facility modernization ($15M GPP)

Multiple investments are required to modernize the APS area of the site to assure that several mission-critical facilities – APS, CNM and the Argonne Protein Characterization Facility – can continue to function as 24-7 scientific user facilities. The main support facilities and utility distribution are original, installed about 25 years ago. Much of the cooling and electrical equipment has reached the end of its life and parts are becoming unavailable as emergency repairs increase. The roofs of all the original facilities also are aging, and leaks and water infiltrations are increasing. We propose to use Argonne repair funds for roof replacements during the APS Upgrade shutdown. Direct funding is required to replace the primary cooling system and the underground piping and electrical distribution. Currently, these assets are direct buried; the proposed modernization would place these critical items in utility tunnels to avoid future failures due to corrosion.

Building 350 legacy project and renovation ($49M SLI, $8.9M GPP)

In FY17, DOE transferred operational responsibilities for Building 350, formerly the New Brunswick Laboratory, to Argonne. To make the building usable for future programs, we have initiated an SLI-funded project to de-inventory about 20,000 nuclear reference materials, clean out hazardous materials, and characterize the residual contamination. A parallel effort to renovate the facility is required to make it useable for research and radiological support operations.
BROOKHAVEN NATIONAL LABORATORY

Lab-at-a-Glance

- **Location:** Upton, NY
- **Type:** Multi-program Laboratory
- **Contractor:** Brookhaven Science Associates
- **Site Office:** Brookhaven Site Office
- **Website:** www.bnl.gov

**Physical Assets:**
- 5,322 acres and 316 buildings
- 4.85 million GSF in buildings
- Replacement Plant Value: $5.23B
- 95,702 GSF in 11 Excess Facilities
- 0 GSF in Leased Facilities

**Human Capital:**
- 2,618 Full Time Equivalent Employees (FTEs)
- 121 Joint Faculty
- 122 Postdoctoral Researchers
- 140 Graduate Students
- 203 Undergraduate Students
- 2,594 Facility Users
- 2,134 Visiting Scientists

**FY 2016 Costs by Funding Source ($M):**

- **NP** $198.3
- **BER** $72.6
- **BES** $202.7
- **HEP**
- **ASCR** $0.6
- **EERE**
- **EM** $0.4
- **NE** $2.6
- **NNSA** $13.4
- **DHS** $1.3
- **Other DOE** $3.9
- **SPP** $50.0
- **Other SC** $15.6
- **EM** $0.4
- **EERE** $4.2
- **NE** $2.6
- **NNSA** $13.4
- **DHS** $1.3
- **Other DOE** $3.9
- **SPP** $50.0

**Mission Overview**

Brookhaven National Laboratory (BNL) brings expertise and world-class facilities to bear on the most exciting and important questions in science—from the birth of the universe to the sustainable energy technologies of tomorrow.

BNL advances fundamental research in nuclear and particle physics to gain a deeper understanding of matter, energy, space, and time; applies photon sciences and nanomaterials research to solve energy challenges of critical importance to the Nation; and performs cross-disciplinary research on computation, sustainable energy, national security, and earth’s ecosystems. Established in 1947, BNL brings unique strengths and capabilities to the Department of Energy (DOE) laboratory system as the only multi-program Laboratory in the Northeast. BNL produces transformative science and advanced technologies, and does it safely, securely, and environmentally responsibly, with the cooperation and involvement of the local, state, and international scientific communities.

With a long-standing expertise in accelerator science and technology, BNL conceptualizes, designs, builds, and operates major scientific facilities in support of its DOE mission. These facilities serve DOE’s basic research needs and reflect BNL/DOE stewardship of national research infrastructure critical for
university, industry, and government researchers. The Relativistic Heavy Ion Collider complex, the National Synchrotron Light Source II, the Center for Functional Nanomaterials, and the Accelerator Test Facility serve more than 2500 scientists/year. Seven Nobel Prizes have been awarded for discoveries made at BNL.

BNL’s strong partnerships with Stony Brook University, Battelle, and the Core Universities are important assets in accomplishing the Lab’s missions. Beyond their roles in Brookhaven Science Associates, Stony Brook and Battelle are key partners in all of BNL’s strategic initiatives, from basic research to the commercial deployment of technology. They underpin BNL’s growing partnerships in the Northeast, especially its vital relationship with New York State.

Core Capabilities

Thirteen core technical capabilities underpin activities at Brookhaven National Laboratory. Each of these core capabilities is comprised of a substantial combination of facilities, teams of people, and equipment that has a unique and often world-leading component and relevance to national needs, as well as to the education of the next generation of scientists from grades K – 12 through graduate school. These core capabilities enable BNL to deliver transformational science and technology that is relevant to the DOE/Department of Homeland Security (DHS) missions, as listed in Appendix A.

1. Accelerator Science and Technology

Summary: BNL has long-standing expertise in accelerator science that has been exploited in the design of accelerators around the world, beginning with the Cosmotron in 1948 and now including RHIC and NSLS-II. Among the now “standard” and widely-used technologies developed at BNL are the strong-focusing principle and the Chasman-Greene lattice, which were transformational developments for modern accelerator and synchrotron light source facilities, respectively. With the construction of National Synchrotron Light Source II (NSLS-II), the Laboratory began adopting high energy accelerator technology to achieve unprecedented brightness, integrating damping wigglers in a unique configuration. NSLS-II is now operational.

BNL’s development and implementation of stochastic cooling for high-energy bunched beams has enabled an earlier and much less costly completion of the Relativistic Heavy Ion Collider II (RHIC-II) luminosity upgrade, enhancing RHIC heavy-ion collision luminosities by approximately an order of magnitude. BNL’s pioneering development of the acceleration of spin-polarized proton beams to high energy using Siberian snakes made RHIC the world’s only polarized proton collider and allows for the unique exploration of the polarization of quarks and gluons inside the proton. The Lab’s developing competencies in superconducting RF technology for high intensity beams, high-brightness high-energy Energy Recovery Linacs (ERL), and innovative electron cooling techniques, together with its established world-leadership in acceleration of spin-polarized proton beams to high energy and high-brightness electron storage rings, lay the groundwork for eRHIC, a future Electron-Ion Collider (EIC) using the RHIC facility. The ERL development is also relevant for possible future high power and high brightness X-ray Free Electron Lasers. World-leading expertise in designing and building high field magnets, including those using high temperature superconductor technology, is essential to upgrades of existing hadron colliders and to the possible construction of future circular colliders.

BNL operates the Accelerator Test Facility (ATF), a unique national user facility for beam physics experiments and technology demonstrations, which also provides training for the next generation of accelerator scientists in cutting-edge tests of advanced accelerator concepts. The ATF is the flagship facility of the DOE Accelerator Stewardship Program within the Office of High Energy Physics (OHEP). An

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2 Columbia, Cornell, Harvard, MIT, Princeton, and Yale
upgrade of the ATF (ATF-II) is in the advanced planning stage. The proposed ATF-II capabilities would provide expanded and more flexible capabilities to a diverse user community that is supported by multiple government agencies as well as industry.

A unique strength of the ATF is the interaction of high-power fast-pulsed lasers with high-brightness electron beams. The development of such lasers at long wavelengths (~10 µm) has led to recent breakthroughs in the generation of mono-energetic ion beams from laser bombardment of gas jets, with game-changing potential for radiotherapy. As a first step of the ATF-II upgrade, the laser power in single pulses would be increased into the 10-20 TW regime, with the ultimate goal of achieving a world-leading 100 TW – a power level that would be transformational for production and acceleration of electron and ion beams.

The Superconducting Magnet Division (SMD) has retained the key elements of expertise used in the design, construction, and test of magnets for RHIC. The high reliability of these magnets has been essential to the superb performance of RHIC. Since the completion of RHIC, the SMD has built smaller numbers of novel magnets that have contributed to the extension of RHIC’s physics capability. Magnets with coils in the form of helices have enabled the collisions of polarized proton beams. A recent increase in the luminosity of RHIC was made possible by the construction of precise solenoid magnets for the electron lens system. The SMD is enhancing a computer-driven coil winding facility that allows multilayer coils with complex windings to be built. Such coils are needed to meet the demands of the magnets that will focus the eRHIC electron and ion beams at the point where they collide.

The SMD has also made significant contributions to other accelerators. The SMD recently deployed its expertise in the precise measurement of the magnets for NSLS-II. The SMD built magnets for the Large Hadron Collider (LHC) at CERN, using a design that closely followed that of the RHIC dipoles. The SMD is working with FermiLab and Lawrence Berkeley National Laboratory to build magnets for the high-luminosity upgrade of the LHC. Magnets have been made at the computer driven winding facility for accelerators in Germany, Japan, China, and an experiment at CERN. The SMD is building a high field magnet using high temperature superconductor cables for a physics experiment that will search for new fundamental particles (axions). The focus of magnet production in the years 2017–2023 will be coil production and magnet testing for the LHC upgrade. The main focus of magnet development during that time will be design, production, and testing of superconducting magnets that focus the eRHIC beams. As the work on magnets for the LHC upgrade nears completion, work on eRHIC magnets is expected to move from development to production in the years 2023-2026.

BNL possesses strength as a world-class accelerator laboratory, which is the foundation of the Laboratory’s and DOE’s research programs. The Lab is pursuing stronger integration of the Accelerator Science and Technology (AST) effort to foster cross-fertilization between the accelerator R&D effort towards eRHIC and the advanced acceleration R&D at the ATF under the Nuclear and Particle Physics Directorate, and the high brightness photon R&D effort under the Energy and Photon Sciences Directorate. AST drives, both internally and externally, the projects currently envisioned to sustain the Laboratory, simultaneously exploiting and reinforcing the creativity, breadth, and flexibility of BNL’s expertise in this area. This includes collaboration with industry for improved ion beam therapy facilities utilizing BNL expertise in developing synchrotrons and Fixed-Field Alternating Gradient (FFAG) accelerators for nuclear and particle physics projects. In addition, a joint project with Cornell University to construct a prototype multi-pass high current ERL with FFAG recirculation arcs is funded by New York State. This project aims to demonstrate a key technology to enable a linac-ring based EIC.

In order to extend BNL’s strong tradition of creative accelerator design well into the eRHIC era, the joint BNL-Stony Brook University (SBU) Center for Accelerator Science and Education (CASE) was established. The mission of CASE is to educate and train the next generation of accelerator scientists and technologists, who will support the growing needs of BNL and the community at large. About ten Ph.D. students are engaged in accelerator research at BNL under the auspices of CASE.
The Office of Nuclear Physics (NP) [mission areas Office of Science (SC) 30, 32], the Office of Basic Energy Sciences (BES) [mission area SC 10], and OHEP [mission areas SC 24, 25, 26], as well as SBU, New York State Energy Research & Development Authority (NYSERDA), and Laboratory Discretionary Funds are the primary sources of funding for the ongoing Accelerator Science and Technology efforts.

2. Advanced Computer Science, Visualization & Data

**Summary:** BNL science is dominated by data rich experimental facilities, such as RHIC, NSLS-II, and the Center for Functional Nanomaterials (CFN) as well as support of others, e.g., ATLAS and the Atmospheric Radiation Measurement (ARM) Facility. Driven by the requirements of these facilities, BNL developed a long-standing research, development, and operational program in advanced computer science and data science methods, algorithms, tools and infrastructures – making it today the largest data science lab in the DOE complex. In 2015, BNL established the Computational Science Initiative (CSI), integrating its many outstanding capabilities under one umbrella.

A core focus of CSI is the continued development of novel data analysis and visualization paradigms in support of data-based discovery at large scale experimental, observational and computational facilities. CSI is driving a paradigm shift, by developing new methods, tools and infrastructures that will enable scientists to analyze and interpret their scientific results as they are emerging during experiments, observations and/or computational modeling. This, in turn, will allow scientists to steer and optimize their research more effectively towards new discoveries. BNL is following a co-design approach in its research, pursuing areas from novel hardware design to highly scalable data analytics methods, with an aim to create integrated end-to-end solutions with measurable impact on scientific discovery cycles. Key strengths are the development of fast and reliable I/O and data transfer mechanisms, new programming models for data intensive computing applications, data intensive workflow requirements, scalable and incremental machine learning, visual analytics-supported decision making environments and provenance for reproducibility, and performance analysis. Two new research areas are: “Analysis on the Wire”, where the network is used as a high throughput computer for high volume, high velocity, highly correlated data analytics, combining BNL’s strength in network and machine learning; and “White Box Machine Learning”, where visual analytics and machine learning are integrated to enable the training and validation of machine learning algorithms.

In support of data intensive computing, BNL has built the third largest data centric computing laboratory worldwide with over 100 PB of archived data. BNL annually ingests ~35 PB, distributes 37 PB, and processes 400 PB of scientific data, delivering ~200 TB/Day to over 100 data centers across the world. BNL also provides 45 PB of fast disk space. The available storage capacity is connected via a 3 Terabits/s network infrastructure to BNL’s extensive data analytics and high performance computing infrastructure. In 2016, BNL hosted 250 racks with ~70,000 cores of high throughput data analysis resource. Next to operating its 3.5 rack Blue Gene Q High Performance Computing resource – 3584 nodes, 64,512 cores, BNL acquired a 108 node Institutional Cluster, each node with 36 Broadwell CPUs and 2 K80 GPUs, to support numerical modeling and novel data analysis development. BNL started its Novel Data-Intensive Architecture Testbed Facility with a 144 node Knights Landing-based system with Dual Rail Omni-Path, in support of research into co-designing new data intensive-computing solutions. A 200 GB/s network link connects BNL to ESnet, which is expected to be upgraded to 300 GB/s in the coming year.

In 2017, BNL is set to expand its computing capabilities through the purchase of a US Quantum Chromodynamics (QCD) system, a doubling of the institutional cluster, and a second data intensive novel architecture system. BNL’s computing infrastructure is supporting ~1700 active users. New service developments in the past year include: the BNLBox, a tool to provide a universal data back-up, storage and sharing service accessible from any device on site and anywhere in the world; and Invenio/Zenodo-based service for the long term management and sharing of data, publications and software, which can host and be customized for a number of communities in parallel.
BNL’s high-throughput data capabilities are leveraged by the RHIC-ATLAS Computing Facility (RACF) that has been delivering, cost-effective computing to both RHIC (NP) and ATLAS (HEP) for the past 15 years. RACF provides ~90% of the computing capacity for PHENIX and STAR data analysis. The ATLAS Tier-1 facility is the largest Tier-1 center worldwide and contributes 23% of the worldwide computing capacity to ATLAS data analysis at 99% service availability. BNL’s expertise in large scale data management has established the BNL ATLAS Center as the most important ATLAS data repository besides CERN. Together with the Physics Application Software group, these resources and capabilities make BNL one of the largest Big Data/High Throughput Computing resources and expertise pools in U.S. science.

The primary sources of funding for this core capability come from OHEP [mission areas SC 21, 22, 24, 26], NP [mission areas SC 27, 30, 32], the Office of Advanced Scientific Computing Research (ASCR) [mission areas SC 2-6], Office of Biological and Environmental Research (BER) [mission areas SC 12, 13, 15, 16], and BES [mission areas SC 7-11], as well as Advanced Research Projects Agency-Energy (ARPA-E) and Laboratory Discretionary Funds. In addition, CSI received New York State funding in support of data-driven discovery research and underpinning hardware purchases.

3. Applied Materials Science and Engineering

*Summary:* BNL engages in a broad range of activities related to energy storage and grid, including materials synthesis, characterization and functional electrochemical evaluation, high energy density cell technology, evaluation of thermal stability and functional limits of battery materials, and fundamental studies of charge and discharge mechanisms and associated material-structure evolution.

BNL has well-established expertise and capabilities for *in situ* characterization of energy storage materials by X-ray methods, and is establishing new capabilities for nanoscale imaging using micro-electrochemical cells for X-ray and electron microscopy under *operando* conditions. These capabilities are used to understand complex active electrochemical interfaces and to carry out research in high energy density cell technology.

BNL has established itself as an important player in grid modernization, focused on the challenges of New York State and the Northeast. BNL is supporting New York State’s efforts to restructure its electricity markets under its “Reforming the Energy Vision (REV)” initiative. BNL is a member of the Grid Modernization Laboratory Consortium and plays a key role in several of the Consortium’s projects. BNL is the lead Laboratory for the DOE regional effort on technical assistance to New York State in support of the REV initiative, in collaboration with other DOE laboratories, and has on-going efforts with utilities in New York and the Northeast.

BNL also has capabilities to study materials in extreme environments for nuclear applications. BNL has developed a specialized robotic system at NSLS-II for the rapid characterization of materials damaged in high-radiation environments, such as pressure vessel steels. BNL is using this capability to provide industry with unique information on the performance of advanced materials for nuclear applications. BNL has also developed a unique end station cell for *in situ* characterization of reactor material under high temperature and pressure. This cell is used to develop new insights on accelerated corrosion of advanced cladding materials for nuclear applications. BNL is the lead on synchrotron characterization of waste forms in a new Energy Frontier Research Center (the Center for Hierarchical Waste Form Materials led by the University of South Carolina) and will leverage NSLS-II in this research.

The BNL Linac is used to support the development of new materials for advanced nuclear reactors. The 200 MeV proton beam of the Linac, the Brookhaven Linac Isotope Producer (BLIP) target facility, and the Tandem accelerators are used extensively for studies of radiation damage in materials for high-energy particle accelerator elements, such as pion production targets for neutrino experiments.

The primary sources of funding are: BES [mission areas SC 7-10], the Vehicle Technologies Program of the Office of Energy Efficiency and Renewable Energy (EERE) [mission area Energy Security (ES) 15], the Office of Energy Delivery and Energy Reliability, [mission area (ES) 10], the Office of Nuclear Energy (NE) [mission areas NE 1, 4], New York State and Laboratory Discretionary Funds.
4. Biological Systems Science

*Summary:* The goal of BNL’s programs in biology is to develop a quantitative understanding of complex biological systems, relevant to the DOE mission with respect to energy and the environment. Expertise ranges from investigating structures of individual proteins, protein complexes, regulation of carbon fluxes from carbon capture, conversion within central metabolism and storage as reduced carbon compounds including lipids and biomass. In all cases, the objective is to create foundational knowledge that relates structure and function, so that desired manipulations, such as increasing growth rates, altering metabolic pathways to enable the accumulation of desired products, or environmental adaptation can be optimized. The tools used include structural biology in a wide variety of forms, molecular biology, physical biochemistry, and biological imaging, which employ a close coupling of experiments with modeling and simulation.

BNL’s Quantitative Plant Science Initiative (QPSI), launched in FY 2016, addresses the grand challenge of “enabling predictive biology.” One key focus area will be on plant genomic dark space, *i.e.,* to accelerate discovery of the large numbers of genes for which there is currently little or no knowledge of function. A key new capability, a genotype-to-phenotype discovery platform, is under construction that will enable genome-wide screening to define the roles of genes in core plant metabolism. Use of this new capability is key to developing the knowledge base needed to model plant processes in order to identify strategies for manipulating living systems to accumulate feedstocks for fuels and other desired products.

QPSI also leverages the newly commissioned world-leading analytical capabilities at NSLS-II, in addition to existing capabilities within the CFN to probe molecular structure and dynamics at unprecedented spatial and temporal resolutions. Using the beamlines at NSLS-II, cryo-electron microscopy (cryo-EM), and fluorescence resonance energy transfer, BNL will perform structural analysis on complex biological systems at scales ranging from angstroms to the whole plant level. BNL will also expand its capabilities for using transcriptomics, metabolomics, fluxomics and proteomics to develop and test detailed plant models so that prediction of behavior *in silico* can become a reality.

The bioinformatics and computational biology capability is an integral part of the BNL biological systems program. BNL researchers contribute to the Systems Biology Knowledgebase (KBase) development team (led by Argonne, Lawrence Berkeley, and Oak Ridge National Laboratories).

BNL has a combination of strong existing programs in plant physical biochemistry and an emerging capability in systems and synthetic biology. In summary, BNL is expanding its efforts in plant biology to include genome-wide functional discovery, modeling, simulation, and computation to position the Lab in a prominent leadership position with regard to Quantitative Plant Science.

Funding comes from BES [mission area SC 10], the Office of Biological and Environmental Research (BER) [mission areas SC 12, 15], a Joint Genome Institute Community Science Program (Gene Synthesis), ASCR and National Nuclear Security Administration (NNSA)/Advanced Scientific Computing Exascale Computing Project [mission area SC 2, 3], the National Institutes of Health (NIH), a Cooperative Research and Development Agreement (CRADA), and Laboratory Discretionary Funds.

5. Chemical and Molecular Science

*Summary:* In chemical and molecular sciences, BNL focuses on basic and applied research in catalytic chemistry for energy conversion processes and fundamental studies in chemical dynamics and radiation chemistry.

Catalysis research builds on a synergistic approach that combines leadership in *operando* studies of powder catalysts, *in situ* studies of model nanocatalysts, and quantum chemical computation. *Operando* studies using synchrotron methods are now exploiting the world-leading capabilities at NSLS-
II. New in situ imaging capabilities based on ambient pressure scanning tunneling microscopy and ambient pressure infrared reflection absorption spectroscopy are transforming the ability to characterize the catalytic active site and its interaction with reaction intermediates in model catalysts synthesized on nanostructured single crystals. These capabilities are being applied to important new energy conversion reactions, such as activation of abundant methane feedstocks to synthesize fuels and chemical intermediates, and sustainable methanol synthesis from small molecules H₂ and CO₂. Expertise in inorganic molecular catalysts is applied to understand and improve chemical processes that underlie solar-to-fuels conversion in artificial photosynthesis. Electrocatalysis research builds on world leadership in synthesis and characterization of nanostructured core-shell metal and metal oxide electrocatalysts.

In chemical dynamics, BNL scientists are leaders in the development of advanced, time-resolved laser spectroscopy methods for characterization of molecular dynamics in gas and condensed phases. All efforts combine leading experimental capabilities with computational methods in quantum molecular dynamics.

The radiation chemistry program benefits from the advanced pulse radiolysis capabilities at the Accelerator Center for Energy Research (ACER). Within ACER, the Laser Electron Accelerator Facility provides capabilities for ultrafast pulse radiolysis, a Van de Graaff accelerator supports kinetics studies on slower timescales, and two ⁶⁰⁰C sources enable irradiation studies. ACER is developing time-resolved infrared spectroscopy as a unique chemically specific probe. Instrumental capabilities involve new quantum cascade laser sources and broadband step-scan Fourier transform infrared instrumentation that are transforming the ability to investigate chemical mechanisms using pulse radiolysis. This is enabling the investigation of chemical mechanisms in photocatalysis, radiation chemistry, and molecular charge transfer and transport.

Fundamental chemistry programs are funded by BES [mission areas SC 7-9, 11] and Laboratory Discretionary Funds, whereas applied fuel-cell electrocatalysis and battery-materials research is supported primarily by EERE’s Hydrogen and Fuel Cells Program [mission area ES 3] and EERE’s Vehicle Technologies Office [mission area ES 15], respectively.

6. Chemical Engineering

**Summary:** BNL has a small but emerging effort in applied chemical research that translates scientific discovery into deployable technologies. BNL has developed innovative catalysts that have the potential to solve problems of low energy-conversion efficiency and high platinum loading in fuel cells. These catalysts contain smaller amounts of precious metal than conventional ones, facilitating commercial applications of fuel cells, including in electric vehicles. Scale-up of some materials is underway with industry partners.

The Synchrotron Catalysis Consortium (SCC), an open organization of current and future users of NSLS-II, will continue to offer opportunities for advanced characterization and testing of real-world catalysts to researchers from universities, industry, and other National Laboratories. New efforts under the Laboratory’s in situ characterization theme will expand SCC efforts across multiple photon science and nanoscience capabilities.

These programs are funded by BES [mission area SC 7-9, 11], the EERE Hydrogen and Fuel-cells Technologies program [ES 3] and through a CRADA with General Motors Corp.

7. Climate Change Sciences and Atmospheric Science

**Summary:** BNL’s atmospheric and terrestrial ecosystem science efforts aim to develop process-level insight into the role of aerosols and clouds on Earth’s climate and the response of ecosystems to a changing climate. BNL researchers are advancing the understanding of interactions along the aerosol-
cloud-precipitation continuum and their impacts on climate for the Atmospheric Systems Research Program. Research focuses on analysis of data gathered from the Atmospheric Radiation Measurement (ARM) Climate Research Facility; studies of the lifecycle and radiative properties of clouds and aerosols; and developing cutting-edge retrievals of cloud properties and processes from remote sensing observations. BNL scientific staff supports the ARM facilities as instrument mentors and as data science specialists, and by making contributions to the design and interpretation of ARM measurements. Climate modeling scientists support the Accelerated Climate Modeling for Energy (ACME) project and the Climate Model Development and Validation (CMDV) program through their expertise in component development, model evaluation, and the strong observational component they bring to these efforts.

Leveraging long-standing support by BER’s Climate and Environmental Science Division and recent BNL investments in the Computational Science Initiative, BNL has developed new capabilities in support of BER’s needs in environmental data analysis, uncertainty quantification, high-resolution atmospheric modeling, and is developing an integrated assessment capability. There is a need to expand computational resources at BNL to meet the increased demand, including additional hires.

BNL researchers in the Terrestrial Ecosystem Science and Technology group, play a central role in both BER Next Generation Ecosystem Experiments (NGEEs) – NGEE-Arctic and NGEE-Tropics. Research is focused on improving the representation of ecosystem processes in Earth System Models and understanding what drives uncertainty in model structure and parameterization in order to increase the ability to understand and project global climate change. BNL scientists study processes that have a global impact on climate and focus on ecosystems that are poorly understood, sensitive to global change, and inadequately represented in models. They use state-of-the-art techniques to study ecosystem processes across a wide range of scales and biomes.

Funding comes from BER [mission areas SC 6, 13, 15, 16] and Laboratory Discretionary Funds.

8. Condensed Matter Physics and Materials Science

Summary: BNL conducts frontier research in Condensed Matter Physics and Materials Science focusing on new and improved complex, nanostructured, and correlated-electron materials for renewable energy, energy storage, and energy efficiency. This is accomplished through interdisciplinary and tightly coupled research programs in materials synthesis, advanced characterization using a range of experimental techniques, both lab and facility based, and theoretical techniques focused on strongly correlated materials.

A unique tool known as OASIS (a leadership-class capability that combines oxide molecular beam epitaxy, angle-resolved photoemission, and spectroscopic imaging scanning tunneling microscopy), is under development and will be completed in the summer of 2017. OASIS will bring together in one instrument the ability to fabricate thin films and examine their properties in situ using both scanning tunneling microscopy and angle-resolved photoemission.

New capabilities in X-ray scattering and angle-resolved photoemission are being developed to exploit the opportunities afforded by NSLS-II. BNL scientists are engaged as community leaders in new beamline proposals for NSLS-II. Two of these proposals have begun their first phase of development.

BNL’s ultrafast electron diffraction facility is being upgraded to considerably enhance the ability to explore non-equilibrium physics in strongly correlated materials. The upgraded facility will include an optical parametric amplifier and a double tilt sample stage. Both of these tools will make it possible to separate the effects of different degrees of freedom in a strongly correlated material.

BNL’s Center for Computational Design of Functional Strongly Correlated Materials and Theoretical Spectroscopy is developing software that will enable its users to predict the properties of strongly correlated materials. The goal is to make the computer programs widely available to the scientific community.
BNL is the lead institution in the Center for Emergent Superconductivity, an Energy Frontier Research Center (EFRC). This EFRC will end next year and BNL is exploring new focus areas to put forth in a renewal proposal. BNL participates in the Center for Mesoscale Transport Properties, an EFRC led by Stony Brook University, which focuses on mesoscale transport properties in complex systems that are important for energy storage.

BES [mission area SC 7-9, 11] and Laboratory Discretionary Funds are the primary sources of funding for these ongoing efforts.

9. Large-Scale User Facilities/Advanced Instrumentation

Summary: As a key part of its mission, BNL has developed and operates user facilities that individual institutions could not have afforded and would not have had the expertise to develop. In FY 2016, BNL served ~2600 users at its DOE designated user facilities, i.e., ATF, RHIC (including NASA Space Radiation Laboratory [NSRL] and the Tandems), NSLS-II and CFN, as well as additional users at the RACF and US ATLAS Analysis Support Center.

NSLS-II is completing its second year as a user Facility, with eleven beamlines operational, eight in commissioning, and nine under construction. By FY 2018, the total in service will be 28. As of April 2017, NSLS-II was operating at 300 mA, with over 96% reliability year-to-date.

Now in its ninth year of operations in 2016, the CFN completed its most productive year ever by supporting 504 users and contributing to 299 user and staff publications. The facility offers state-of-the-art capabilities for nanomaterial synthesis-by-assembly, and \textit{in situ} and \textit{operando} nanomaterial characterization using optical, electron, and X-ray probes. The CFN is significantly enhancing its ultrafast laser spectroscopy facility, and has recently commissioned a 3D nanoscale lithography instrument. This year, the CFN and NSLS-II will also complete the transition to user operations of four partner endstations that will provide unique nanomaterials characterization by X-ray scattering, spectroscopy, and spectro-microscopy.

BNL envisions an electron-ion collider (eRHIC) as the next major upgrade of RHIC. Such an upgrade would support a new generation of users interested in using high-energy electron-ion collisions to study cold nuclear matter at extreme gluon densities and enable precision measurements of the structure and properties of polarized protons. In addition, BNL researchers and staff support the ARM Climate Research Facility and lead the External Data Center and ARM metadata management. Further, ATF-II has commissioned a new user capability for materials characterization using ultrafast electron diffraction.

BNL also makes important contributions to international facilities – the LHC, and such future facilities as a Long Baseline Neutrino Facility (LBNF)/Deep Underground Neutrino Experiment (DUNE) and the Large Synoptic Survey Telescope (LSST), which is under construction. This core capability is strongly tied to those in \textit{Accelerator Science and Technology, Advanced Computer Science, Visualization & Data, and Systems Engineering and Integration} [CC 1, 2, 13].

The Long Island Solar Farm (LISF) is creating the largest data set (solar insolation, weather, power, and power quality) for a utility-scale solar plan in the U.S. Such data represents a unique asset to study and improve solar forecasting models for utility operations in systems with high levels of solar energy penetration.

The Instrumentation Division supports projects and research programs at major scientific user facilities by conceptualizing, designing, and constructing state-of-the-art detectors, electronics, and optical and laser systems used in the experiments. BNL staff has designed and constructed or helped to construct...
instruments for use at RHIC, NSLS-II, FermiLab, LHC, LSST, the Spallation Neutron Source, the Los Alamos Neutron Scattering Center, the Linear Coherent Light Source, and other accelerator- and reactor-based facilities around the world. The Division is known for its leadership in noble liquid detector technology, low-noise electronics, application specific integrated circuit (ASIC) design, state-of-the-art silicon and neutron detectors, development of high brightness electron sources, and design of metrology systems for measuring synchrotron beamline optics. The Division is pioneering new photocathode development for low energy RHIC electron cooling and for coherent electron cooling. The Division is also pioneering the application of diamond detectors for synchrotron radiation, especially those that are capable of measuring beam position, flux and profile simultaneously, a unique new tool for NSLS-II. Diamond detector applications in diagnostics for proton and ion beam medical therapy are now under study. BNL has wide experience with the construction of gamma-ray spectrometers, neutron imaging and directional detectors, as well as long-range detection of special nuclear materials for national security applications.

The major sources of funding are: BES, NP, HEP, BER [mission areas SC 10, 16, 24, 25, 26, 30, 32], Case Western Reserve University, the Department of Commerce, the Department of Homeland Security (DHS) [mission area Homeland Security (HS): 2], the National Aeronautics and Space Administration (NASA), NNSA [mission area National Security (NS) 2], New York State, the New York Structural Biology Center, NIH, and Laboratory Discretionary Funds.

10. Nuclear & Radio Chemistry

Summary: BNL’s nuclear science programs span the range from applications in medicine to national security. At the Brookhaven Linac Isotope Producer (BLIP), BNL plays a critical role in preparing radioisotopes for the nuclear medicine community and industry that are unavailable commercially. BLIP is one of the world’s major sources of Sr-82, the parent of Rb-82. This short-lived positron emitter is Federal Drug Administration-approved and used routinely for assessment of cardiac function following a heart attack and in diagnosis of coronary artery disease in more than 300,000 patients per year. This work continues BNL’s long leadership tradition in radiotracer development.

To bolster BNL’s leading role in developing and producing radioisotopes through the Medical Isotope Research and Production program, the Lab will increase the quantities of isotopes produced for cancer diagnostics and therapies. The strategic R&D vision focuses on developing radioisotopes or radioisotope pairs that combine both emission of imaging photons and alpha or beta particles for therapy. The highest priority, in collaboration with Los Alamos and Oak Ridge National Laboratories, is the development of an accelerator route to produce Ac-225, an alpha emitter with high potential for cancer therapy, especially for difficult diffuse cancers. Ac-225 has the ability to destroy cancer cells more precisely, without damaging healthy surrounding cells. However, its production elsewhere has been costly and too limited to support clinical trials based on the isotope. Those shortages of Ac-225 could be significantly lessened by this research. Using high-energy proton beams to irradiate thorium targets at BLIP, BNL researchers demonstrated that the current annual supply of Ac-225 can potentially be produced in a week. A Linac beam current upgrade and the installation of a beam raster at BLIP have enhanced its capability. BLIP also supports an active program of radiation damage studies of interest to FermiLab, the Facility for Rare Isotope Beams, the European Spallation Source, KEK, and LHC and for future high power accelerators. A doubling of the Linac beam current for radioisotope production and addition of a second beamline and target station were recommended by the 2015 Nuclear Science Advisory Committee-1 report for BLIP and are also under consideration in the future.

BNL’s expertise in accelerator development has led to a patent for a Rapid Cycling Medical Synchrotron and for low-mass beam delivery gantries, viewed as technologies of choice for the next generation of proton- and ion-based cancer therapy centers. BNL has established a CRADA with a commercial partner interested in building such next-generation centers.
BNL has leading expertise in the application of ionizing radiation for the diagnosis and treatment of cancer. The effects of ionizing radiation on living systems are studied at the NSRL, a flagship international user facility supported by NASA. The NSRL facility also provides the unique capability to study the effectiveness of using carbon or other ion beams for cancer therapy. The Lab is collaborating in developing corresponding research proposals to the National Cancer Institute. NSRL is uniquely positioned to study the effects of exposure of materials and electronic components used in satellites and instrument to cosmic rays. BNL Management is in discussions with NASA about the modality of a user program at the NSRL, which would allow users supported by other funding sources equitable access to the facilities.

The Lab’s nonproliferation and national security programs offer a wide range of skills that include scientific and technical participation in the NNSA Radiological Assistance Program (RAP). BNL supports RAP’s planned deployments to secure national government, sporting, political, and cultural events and unplanned deployments to provide radiological support to local, regional, and tribal governments and private industry. BNL also assists NNSA and DHS efforts to test and evaluate candidate hand-held and unattended systems for prevention of and response to nuclear and radiological events, domestically and abroad.

BNL has extensive expertise in nuclear nonproliferation and international nuclear safeguards that includes forty years of program management for the International Safeguards Project Office (ISPO) for the U.S. Support Program (USSP) to International Atomic Energy Agency (IAEA) Safeguards. ISPO is responsible for coordinating all U.S. technical and personnel support provided through the USSP to the IAEA’s Department of Safeguards. BNL also develops curricula and provides safeguards implementation training for IAEA inspectors and officials from other countries where IAEA safeguards are applied and provides input to technical and policy papers for the NNSA and other sponsors. Applying its expertise with detector materials, BNL is working with FLIR Radiation Inc. to improve the detection capabilities of the R200 handheld radiation detectors.

BNL’s research in the development of improved cadmium zinc telluride (CZT) prototype radiation detectors and imaging arrays is internationally recognized. BNL’s efforts are primarily directed towards nonproliferation and homeland security applications, but are also being applied to medical uses for early detection of cancer. This world-class capability includes facilities for growing, fabricating and characterizing semiconductor and scintillator crystals, designing the ASICs, and assembling and testing the radiation detector prototypes for incorporation into instruments. BNL synthesizes, purifies, and grows CZT and related ternary and quaternary compounds in-house, and serves as an R&D hub for analysis of materials and detectors provided by other institutions. The program has used the CFN for its synthesis efforts and NSLS-II and the Advanced Light Source for its characterization efforts and benefits from the Condensed Matter Physics and Materials Science core capability (CC 8). BNL also assists industry by evaluating commercially available detector materials.

Using position-sensitive $^3$He pixeled detectors fabricated by the Instrumentation Division, BNL has developed unique coded-aperture thermal-neutron imaging systems for arms control treaty verification and counterterrorism applications. One such system was prepared for the Warhead Measurement Campaign to acquire radiation signatures from stockpiled nuclear weapons. BNL participated in long-range stand-off neutron imaging exercises, collaborating with Idaho and Argonne National Laboratories and the Remote Sensing Laboratory. BNL also developed a high-bandwidth system for data acquisition from correlated gamma and neutron events that are indicative of fission chains, and demonstrated expertise in modeling of radiation transport and simulating the response of these measurement systems.

BNL staff members have twenty years of experience in nuclear security analysis and technology from their involvement in the NNSA Materials Protection Control and Accounting program (MPC&A). This
capability is now in demand by other countries, where there are similar nuclear material security concerns. BNL is using the experience amassed through MPC&A and ISPO to assist IAEA member states in understanding and meeting their commitments under the Nuclear Nonproliferation Treaty, especially in the Middle East, North Africa, and Southeast Asia. The Department of State’s (DOS) Chemical Security Program is employing BNL for similar skills aimed at the chemical industries in these regions. BNL is also assisting with the construction of a nuclear security training center in Kazakhstan.

Funding in this area comes from several sources, including NP [mission area SC 31], DOS, NASA, NNSA [mission area NS 1, 2], DHS [mission area HS 2, 6], and a CRADA.

11. Nuclear Physics

Summary: BNL conducts pioneering explorations of the most fundamental aspects of matter governed by Quantum Chromodynamics (QCD). Heavy-ion collisions at RHIC probe matter at temperatures and densities representative of the early universe, mere microseconds after its birth. RHIC experiments discovered that the infant universe was filled with a previously unknown type of liquid matter, the quark-gluon plasma (QGP). The QGP produced in RHIC collisions has a lower viscosity, relative to its density, than any other material known and has been called the “perfect fluid.” The RHIC results have led to profound intellectual connections with other physics frontiers, including string theory, the origin of the universe’s matter-antimatter asymmetry, strongly correlated condensed matter systems, fermion gases trapped at nano-Kelvin temperatures, and density fluctuations in the early universe reflected in cosmic microwave background maps. Important upgrades to the RHIC accelerator and detector complex (3-dimensional stochastic cooling, the Electron Beam Ion Source, collision region compressing cavities, electron lenses; DAQ upgrade and Heavy Flavor Tracker in STAR, central and forward Si vertex detectors in PHENIX) are now in place and have allowed RHIC to run at more than 20 times design luminosity since FY 2014. The collider reached 44 times design luminosity in FY 2016. The vertex detector upgrades enabled a robust program of heavy quark measurements during FY 2014-16, which has produced important new results. The completed heavy quark campaign is being followed by a focused campaign in FY 2017-18 on the dynamics of spin in the proton and chiral effects in the QGP. A future low-energy electron beam cooling upgrade, which will allow for precision mapping of the QCD phase diagram, is in preparation for a physics program in FY 2019-20. A major upgrade to the PHENIX experiment to allow for an extensive array of measurements using jets to precisely probe the transport properties of the QGP received Critical Decision 0, in preparation for a multi-year experimental campaign in the first part of the next decade.

Heavy ion collisions, guided by theory, are used: to quantify the transport properties of the QGP and its response to energetic probes, especially jets and heavy quarks: to probe the gluon structure of nuclei at high energy; to study local fluctuations within the QGP corresponding to violations of fundamental symmetries; to search for a predicted critical point in the QCD phase diagram; and to search for fundamental transformations of the QCD vacuum at extreme temperatures. Collisions of polarized protons, both with themselves and, for the first time, on unpolarized heavy ions in FY 2015, uniquely available at RHIC, are used to elucidate the spin structure of the proton and the yet largely unexplored dynamics of spin degrees of freedom in QCD.

The dramatically improved luminosity and the enhanced detector capabilities of RHIC have enabled a series of recent surprising scientific discoveries. These include: the discovery that a substantial part of the proton spin is carried by gluons; that quark-gluon plasma droplets as small as a single proton can exhibit the characteristic near-perfect fluidity (the unique ability of RHIC to accelerate and collide protons, deuterons and $^3$He nuclei with large nuclei, such as Au, were critical in this demonstration); the first measurement of the force between two antiprotons; and the first measurement of global hyperon polarization in heavy ion collisions, which is sensitive to the vorticity of the fluid. First measurements from the FY 2014-16 heavy quark program show, with unprecedented precision, that the charm quark
participants surprisingly strongly in the collective flow of the quark-gluon plasma.

RHIC offers a synergistic environment for collaboration with universities, other National Labs, and industry. To date, the RHIC program has produced more than 300 Ph.D. nuclear physicists. Nuclear theory efforts at BNL and throughout the international theory community guide and stimulate planning and interpretation of RHIC experiments. They include world-leading programs in high-temperature lattice QCD simulation and the theory of QCD matter at high gluon density.

Experimental, theoretical, and computational research is enhanced by the presence of the RIKEN BNL Research Center (RBRC). In addition to its contributions to the RHIC research program and its role in facilitating scientific collaboration with Japan, the RBRC continues to have a major role in the development of the U.S. nuclear science workforce by helping to establish faculty positions at leading research universities (121 fellows and post docs to date, 90 are associate and assistant professors, of which 60 are tenured).

BNL develops advanced software and computing facilities for applications in nuclear physics experiments and theory. Key expertise has been developed in the management and processing of petabyte-scale data sets generated at high rates and distributed computing for analysis, facilitated by the RACF. Lattice QCD simulations utilize high performance computing facilities at BNL (the Blue Gene/Q machines), as well as at leadership class computing facilities to explore theoretically the phase diagram of QCD.

Future addition of an electron accelerator could convert RHIC into an Electron-Ion Collider (EIC) that would facilitate quantitative study of a regime of saturated gluon densities, present in all ordinary matter and featuring the strongest fields in nature. BNL scientists, in conjunction with Thomas Jefferson National Accelerator Facility (JLab), are leading a national effort to develop the science agenda for a future EIC facility, for which the BNL plan, called eRHIC, is to upgrade the RHIC facility with a high energy electron beam to collide with the existing heavy ion and polarized proton beams. BNL administers a DOE-funded, peer-reviewed R&D program to support universities and Laboratories in the development of advanced instrumentation technologies for an EIC detector, which has provided to projects selected by the program $7.5M since the program’s inception in 2011.

Development and enhancement of RHIC accelerator facilities benefits from a first-rate program of advanced accelerator R&D (see CC 1), while enhancement of the RHIC detector capabilities benefits from the BNL support of the Instrumentation Division (see CC 9).

BNL maintains a world-leading nuclear theory group whose research is focused on the dynamics of relativistic heavy ion collisions and properties of QCD matter at high temperature and density. In 2016, BNL was named as lead institution for two Topical Collaborations in Nuclear Theory, called “Coordinated Theoretical Approach to Transverse Momentum Dependent Hadron Structure in QCD” and the “Beam Energy Scan Theory Collaboration,” respectively. In 2017, B. Schenke was awarded the Zimanyi Medal, a high profile award.

BNL operates the National Nuclear Data Center (NNDC), an international resource for the dissemination of nuclear structure, decay, and reaction data that serves as the focal point for the U.S. Nuclear Data Program (USNDP) and reactor design. The mission of the USNDP is to provide current, accurate, authoritative data for workers in pure and applied areas of nuclear science and engineering. This is accomplished primarily through the compilation, evaluation, dissemination, and archiving of extensive nuclear datasets. The program also addresses gaps in the data, through targeted experimental studies and the use of theoretical models. Last year, there were over four million data retrievals from the NNDC websites.

Funding is provided by NP [mission areas SC 27, 30, 32] as well as New York State, RIKEN and Laboratory Discretionary Funds.
12. Particle Physics

**Summary:** BNL provides intellectual and technical leadership in key particle physics experiments that seek answers to seminal questions about the composition and evolution of the universe, i.e., the source of mass, the nature of dark matter and dark energy, and the origin of the matter-antimatter asymmetry in the universe. BNL’s major roles are: host institution for U.S. contributions to particle physics with the ATLAS detector at the LHC; leadership in neutrino oscillation experiments, including co-host Lab for the Daya Bay reactor neutrino experiment and host of the International Project Office for DUNE, with leading roles in the short-baseline experiments at FermiLab (MicroBooNE and the Short Baseline Near Detector [SBND]), and the long baseline DUNE (FermiLab to the Sanford Underground Research Facility), to complete measurement of the neutrino mixing matrix, including possible CP-violation; and development of a program of observational cosmology (LSST) and precursor efforts, the Dark Energy Survey (DES) and the Baryon Oscillation Spectroscopic Survey (BOSS).

These roles are enhanced by BNL theory efforts and by BNL’s international leadership in critical detector and advanced accelerator research and development (AARD) for next-generation facilities, including a possible energy-frontier proton-proton collider. Detector R&D at BNL is strongly leveraged by Laboratory support for the Instrumentation Division, which has made world-leading contributions to radiation detectors of various types and to low-noise microelectronics and cold electronics (CC 9). BNL has initiated two phases of physics-motivated detector upgrades to ATLAS for higher luminosity running of the LHC. BNL’s expertise in Nuclear Chemistry provides world-leading development of metal-loaded liquid scintillator materials critical to contemporary neutrino experiments. BNL operates a unique national user facility for AARD, the ATF, largely with OHEP funding (see CC 1). The ATF has recently been designated as the first user facility to advance the goals of the HEP accelerator stewardship program. An expansion and upgrade to the facility has been approved; discussions between BNL and DOE on possible implementation scenarios that best meet the research needs of the user community are ongoing.

BNL develops advanced software and computing facilities for applications in high energy experiments and theory. Key expertise in high throughput computing has been developed in the management and processing of petabyte-scale data sets generated at high rates and distributed computing for analysis, facilitated by the RACF, the Physics Analysis Software group, and US ATLAS Analysis Support Center. Lattice QCD simulations utilize high performance computing facilities that include the augmented Blue Gene/Q (BG/Q) machines supported until the end of September 2017. BNL physicists will continue to explore theoretically the properties of elementary particles using the BNL High Performance Computing Institutional Cluster in FY 2017-18 and evaluate new hardware to replace BG/Q in FY 2018. Particle physics software and computing development for both experiment and theory benefit very strongly from synergies with RHIC facilities funded by Nuclear Physics and with the RBRC, funded by the Japanese RIKEN Institute.

The Higgs boson was discovered at the LHC in data taken mainly in 2011-2012 with strong BNL contributions to construction and operation of the detectors, analysis of the data, and computing. This discovery led to the 2013 Nobel Prize being awarded to François Englert and Peter W. Higgs. ATLAS published first results from the 13 TeV Run 2 data in 2016 and collected record amount of data during 2016 operations. Following the groundbreaking Daya Bay discovery in 2012 of a non-zero sin^2θ_{13}, which established that the electron neutrino is composed of all three neutrino states, Daya Bay published a precision measurement of the neutrino mixing angle θ_{13}. This measurement establishes that the future DUNE measurements of CP-violation are feasible. In 2016, BNL led both the new sterile neutrino limit from Daya Bay as well as the joint analysis with MINOS resulting in a tighter limit on sterile neutrinos. MicroBooNE accumulated more data on neutrino interactions.

Recent high profile awards in Particle Physics are: S. Dawson is a co-recipient of the 2017 APS J.J. Sakurai Prize for her contributions to the physics of the Higgs boson and H. Davoudiasl was elected as an APS Fellow. In addition, Christoph Lehner received a 2016 Early Career Award.
13. **Systems Engineering and Integration**

**Summary:** BNL solves problems holistically and across multiple disciplines on several levels in order to deliver Large-Scale User Facilities/Advanced Instrumentation. Individual facility components (accelerators, detectors, beamlines, etc.) that are conceived, designed, and implemented at BNL are complex entities, requiring broad integration for their successful performance and, in turn, for their coupling with other systems. BNL’s approach applies not only to engineering at the various stages of a single project, but also to developing cutting-edge technologies that fuel multiple large projects at the Laboratory.

One example is BNL’s development of noble liquid detectors from concept, through demonstration, to implementation in major particle physics experiments (D0 at FermiLab and ATLAS at LHC), with continuing R&D aimed at developing the very large liquid argon (LAr) time projection chambers (TPCs) that form the core of MicroBooNE and will serve as the short-baseline near detector (SBND) experiment at FermiLab, and the future deep underground long baseline neutrino experiment (DUNE). The cold electronics developed at BNL for LAr TPCs have been utilized in research and development of other TPCs, including LArIAT at FermiLab and ARGONTUBE at the University of Bern.

A second example involves application of high-brightness electron beam technology developed at BNL to NSLS-II and the proposed future electron-ion collider (eRHIC). A further example is BNL’s integration of leading accelerator, beam delivery, targetry, and radiochemistry expertise at the BLIP Target Production Lab.

BNL’s nuclear energy experts support the development of next generation reactors through research on alternative fuel cycles, materials in extreme environments, and assessment of the role of nuclear energy in our Nation’s energy future. BNL serves as the lead laboratory to the Nuclear Regulatory Commission’s (NRC) multi-year program on the licensing of non-light water reactor policy and technical guidance support. BNL staff members serve as the Light Water Reactor Computational Analysis Technical Area Lead within the Fuel Cycle Research and Development program within the Office of Nuclear Energy (NE). BNL also uses state-of-the-art computer tools to analyze nuclear reactor and fuel cycle designs for DOE, NRC, and the National Institute of Standards and Technology (NIST).

The major sources of funding for this core capability come from BES, HEP, NP, and BER [SC mission areas 10, 11, 21-27, 30-32], NE [mission areas NE 1, 4], NIST, NRC, and Laboratory Discretionary Funds.

14. **Proposed Emerging* Computational Science**

**Summary:** BNL has an exceptional history of harnessing outstanding expertise in computer science and applied mathematics to develop leading high performance computing (HPC) solutions in domains, such as lattice Quantum Chromodynamics (QCD), Materials Science and Chemistry, upon which it is building today. BNL plans to request computational science as a Laboratory core capability in the next one to two years.

At the forefront of BNL’s Computational Science expertise are its lattice QCD groups, where Michael Creutz demonstrated the first computation of this kind in 1980. A highlight of the lattice QCD work is that BNL researchers not only leverage computer science expertise, but also actively influence the field in return. Their QCDSP system was the foundation for a collaborative project to create the QCDOC, a direct forerunner of the IBM Blue Gene series. A BNL team played an integral role in developing the hardware and software for this series. Today high levels of efficiency are achieved by parallelizing physical space-time over MPI, OpenMP, and SIMD layers and the exact treatment of the low-lying eigenspace of the QCD Dirac operator. ASCR-funded research in HPC programming models and interfaces supports strategies for QCD program optimization that will lead to efficient, performance

Funding for this work comes from OHEP [mission areas SC 21-26] as well as RIKEN and Laboratory Discretionary Funds.
portable code on future platforms. A joint BNL CSI and Physics team assesses gaps and problems in existing parallel programming interfaces and contributes to the leadership and development of two directive-based standards efforts, OpenMP and OpenACC, and OpenShmem and multiple other community efforts. In 2016 the BNL CSI and Physics team was instrumental in winning the QCD Exascale Computing Project (ECP) focused on Applications.

Computational Materials Science at BNL dates back to studies of material structure for nuclear science in the 60s and 70s, use of the lattice Monte Carlo method in the 80s and 90s, and density functional theory (DFT) for nanoscience research (2000-2014). In 2015, BNL was awarded the BES Center for Computational Design of Functional Strongly Correlated Materials and Theoretical Spectroscopy. Joint computer science and applied mathematics work focuses on code optimization and performance portability on ASCR Leadership Computing Facilities.

The Pacific Northwest National Laboratory-led NWChemEx ECP comprises a multi-disciplinary team to bring computational chemistry and materials methods to future extreme scale computing systems. Harrison (BNL, Stony Brook University) is the project’s lead architect and van Dam (BNL) is lead for the science use cases and scalability studies. The project focuses on molecular dynamics, DFT and many body methods to tackle problems related to the development of bioenergy crops and catalysis. The ECP Co-Design Center for Online Data Analysis and Reduction at the Exascale (CODAR) collaborates with NWChemEx on exploring online data reduction techniques of structure sequences resulting from extreme scale molecular dynamics calculations.

Novel algorithms and libraries for complex multiphysics and multiscale systems were developed at BNL and implemented in scalable codes. They include: the particle-in-cell electromagnetic code SPACE that implements state-of-the-art algorithms for relativistic particles and fields; the method of Lagrangian particles that greatly improves the accuracy and mathematical rigor of the known method of smoothed particle hydrodynamics; its complement, the Adaptive Particle-in-Cloud method (AP-Cloud), which is a highly adaptive replacement for the traditional Particle-in-Cell method (PIC) that eliminates the traditional mesh; and the FronTier-MHD code, designed for simulations of free-surface and multiphase magnetohydrodynamic flows. All codes have been extensively used for DOE applications.

The primary sources of funding for this emerging core capability come from OHEP [mission areas SC 21, 22, 24, 26], NP [mission areas SC 27, 30, 32], the Office of Advanced Scientific Computing Research (ASCR) [mission areas SC 1-6], Office of Biological and Environmental Research (BER) [mission areas SC 12, 13, 15, 16], and BES [mission areas SC 7-11], as well as Advanced Research Projects Agency-Energy (ARPA-E) and Laboratory Discretionary Funds.

These core capabilities, along with BNL’s proven expertise in large science project management, will enable the Lab to deliver its mission and customer focus, to perform a complementary role in the DOE laboratory system, and to pursue its vision for scientific excellence and pre-eminence.

Science Strategy for the Future

BNL has identified six scientific initiatives that, when achieved, will help realize the vision for the Lab. These are major Laboratory thrusts that align with the DOE Strategic Goals in Science, Energy and Nuclear Security and build on the Laboratory’s core strengths and capabilities. BNL envisions that it will continue to distinguish itself by delivering transformative science, technology, and engineering in these areas that will enable the Laboratory to make the world a better place. BNL envisions inventing new technologies to power the future, unlocking the mysteries of how the universe’s smallest particles interact, and finding solutions for some of our nation’s greatest challenges. In order to reap the potentially transformational benefits of these initiatives, a key element of Brookhaven’s strategy is to pursue the evolution of its two largest user facilities – National Synchrotron Light Source II (NSLS-II) and the Relativistic Heavy Ion Collider (RHIC).
Particular areas of emphasis for BNL are: exploiting RHIC’s capabilities to learn about the matter that makes up nearly all of the visible universe and setting the foundation to transition to an Electron-Ion Collider; working to solve grand challenges in energy that will create solutions and security for the nation’s energy system by leveraging its state-of-the-art facilities; making sense of data at the exabyte-scale and beyond; maintaining leadership in key high energy physics experiments that will lead to a deeper understanding of the composition of the universe; building on its unique combination of accelerator-based facilities and broad technical expertise to support efforts in accelerator science and technology that range from innovations to applications; and developing a quantitative understanding of biological processes relevant to the DOE mission with respect to energy and environment.

These science outcomes are underpinned by two operational initiatives that address essential operational support for the future: a revitalized physical plant to enable the Lab’s science, attract and retain the scientific work force, support the needs of users, and assure the reliable functioning of BNL’s scientific facilities; and safe, secure and efficient operations, which are crucial for the Laboratory to succeed in all that it does.

**Infrastructure**

**Overview of Site Facilities and Infrastructure**

The vision for BNL is structured around the achievement of eight Initiatives, of which six are at the heart of BNL’s vision for science. BNL’s approach to Laboratory operations emphasizes two additional initiatives: a renewed research campus that will enable BNL’s research mission; and safe, secure and efficient operations that ensure delivery of the research mission. The Lab’s approach to mission readiness will provide a revitalized physical plant to improve scientific productivity, promote the attraction and retention of the scientific work force, including the significant BNL user population, and assure the safe, reliable functioning of BNL’s major scientific facilities.

BNL is located in Upton, New York in central Suffolk County approximately 75 miles east of New York City. The BNL site, former Army Camp Upton, lies in both the Townships of Brookhaven and Riverhead. BNL is situated on the western rim of the shallow Peconic River watershed. The marshy areas in the site’s northern and eastern sections are part of the Peconic River headwaters. Approximately 25% of BNL’s 5,322 acre site is developed.

At the end of FY 2016, there were 316 buildings totaling 4,848,736 square feet (sf). All buildings are owned by the DOE Office of Science (SC). Other Structures and Facilities (OSF) assets are owned by SC, except for FIMS Asset ST0704, the High Flux Beam Reactor (HFBR) stack, which remains under the Office of Environmental Management (EM). BNL does not lease any facilities. The average age of all buildings is 45 years. Sixty-four buildings (762,388 sf) date back to World War II (WW-II) and most major permanent science facilities, excluding the Research Support Building, Interdisciplinary Science Building (ISB), former National Synchrotron Light Source (NSLS), National Synchrotron Light Source II (NSLS-II), Relativistic Heavy Ion Collider (RHIC) and the Center for Functional Nanomaterials (CFN), were built in the 1950s and 1960s. Excluding the areas covered under the Renovate Science Laboratories (RSL)-I/II Science Laboratories Infrastructure (SLI) projects and minor work done under General Plant Projects (GPP) and Laboratory-funded projects, these facilities have not received any major renovation and many building systems are well past the end of their economic life and need replacement.

EM has qualified (for acceptance) several shutdown facilities waiting to be decommissioned and decontaminated, subject to available funding. Transfers to DOE-EM from DOE-SC will occur when the projects are funded. Included are the former Brookhaven Medical Research Reactor, Brookhaven Graphite Research Reactor, and HFBR facilities.

In FY 2016, three buildings (B528A, B562, and B580), totaling 1,450 sf, were demolished. In early FY
2017, two building totaling 21,944 were demolished: B180 and a portion of B463, an old greenhouse. At
the end of FY 2016, there were 11 excess buildings totaling 95,702 sf. During FY 2017, B134 with 19,578
sf will be declared excess, as staff members were relocated from this inadequate space to better space
in underutilized buildings as part of BNL’s consolidation efforts. There are also five modular buildings
totaling 15,337 sf connected to non-excess FIMS assets that will be demolished in the future.

In FY 2016 there was 284,613 sf of non-excess, “Not Utilized” (<10% utilized) space in active buildings.
The majority of this space - 156,205 sf (55%) was the former NSLS facility, B725. This space is now
partially occupied and considered utilized. There are plans for further use of this facility. To accomplish
this, indirect funds will be used to renovate office space and an SLI Line Item, the Core Facilities
Revitalization (CFR), which recently received CD-1, will convert most of the former research space to a
computer center with modernized major building systems and a renewed building envelope. The
majority of the remaining “Not Utilized” space is in B750 (former HFBR), for which a small portion
located outside the containment structure is used by the Radiological Assistance Program (RAP). BNL is
investigating relocating RAP so the building can be declared Excess.

The BNL Land Use Plan, being updated in 2017, can be found at:

Campus Strategy

Modern science is enabled through capable and reliable infrastructure. A renewed and well-operated
physical plant improves scientific productivity; promotes the attraction and retention of the scientific
workforce, including the significant BNL user population; and along with the Lab’s operational
excellence, underpins the capability of its scientific facility portfolio. BNL has tailored its campus
strategy to support the programmatic Initiatives, thus enabling the Lab’s research mission. The resulting
strategy consists of four major elements:

• Focus limited DOE investment in critical core buildings and infrastructure to enable the scientific
  agenda
• Make research safe and cost effective by downsizing the campus and demolishing old buildings
• Ensure scientific reliability through targeted investments in buildings and utility infrastructure
• Support the growing population of scientific users through an innovative concept called “Discovery
  Park.”

The BNL Site Master Plan map (Appendix B) shows the location of the key investments of the campus
wide strategy. The proposed capital funding for these investments is indicated in Enclosure 6. The
planned infrastructure investments will promote and support the six scientific Initiatives and the wide
range of facilities that enable BNL’s thirteen core capabilities. In addition, the Laboratory must provide
world-class facilities that will support the recruitment and retention of premier staff.

Since many of BNL’s permanent science buildings are 50+ years old, they require substantial
sustainment and recapitalization investments in mechanical and electrical systems and architectural
elements to meet the demands of modern research methods. Research labs need to be renewed and
modernized to include new fume hoods and casework. In addition, many research labs need state-of-
the-art upgrades, including stringent environmental and vibration controls and “clean” environments.
BNL has identified those “permanent” facilities that will form the platform for current and future core
capabilities. To ensure facilities are mission ready, BNL has formulated a multi-pronged strategy of
consolidation and rehabilitation. Facilities would be rehabilitated using a combination of indirect funds
(Institutional General Plant Projects (IGPP), Deferred Maintenance Reduction (DMR) and DOE direct
funds (SLI, GPP).

The most significant issue facing the support divisions is that many are still located in WW-II era wood
buildings. To address this, the Science and User Support Center (SUSC) is proposed as a modern, signature facility using SLI funding to consolidate support organizations and provide a Laboratory visitor building, training, and user services portal in synergy with the Discovery Park development.

While BNL's utilities are currently reliable, they are aging and issues impacting reliability and capacity are increasing. In FY 2011, BNL completed a baseline study, which evaluated its utilities and recommended strategies to address critical needs. The study identified significant short-term needs confirming that the aging water, electric, chilled water, and steam distribution system components need replacement. Recapitalization resources to renew and replace BNL’s utility infrastructure have been limited by very tight operating budgets. However, progress has been made to increase Central Chilled Water Facility (CCWF) capacity and reliability to support growing science process cooling needs with the installation of new electric centrifugal chillers and a project to replace the 27-year-old wood cooling tower at the CCWF, which will be completed during FY 2017. BNL has also started engineering two potable water projects: one to replace the WWII-era 300,000 gallon elevated water storage tank and one to rebuild Potable Water Well No. 12. Their construction is scheduled to complete in FY 2020 and FY 2022, respectively.

An important element of the overall infrastructure strategy is elimination of excess facilities and footprint reduction to realize operational efficiencies, improved safety of facilities, and improved utilization and quality of space. The Infrastructure Investment Table and Integrated Facilities and Infrastructure (IFI) crosscut reflect both an aggressive program of annual overhead investments to eliminate existing or anticipated future non-contaminated excess facilities as well as funding requests for direct DOE funding for the more costly contaminated facility projects. Over the planning period, it is estimated that over ~287,000 sf of primarily WW-II era buildings will be eliminated.

To meet these infrastructure challenges, BNL has formulated a strategy to address the mission and operational needs based on the constraints and strengths of the various funding sources. Capital projects and other requested funding are shown in the Infrastructure Investment Table and indirect expensed projects, such as DMR are reflected in funding plans shown on the IFI Crosscut, both of which are in Enclosure 6. In addition, there are non-capitalized betterment and alteration projects and infrastructure studies that BNL refers to as Other Infrastructure Projects (OIP), not requested as part of Enclosure 6, that round out the Lab’s investment strategy. Consistent with BNL’s Mission Readiness approach, funding for the various categories of indirect funds (DMR, OIP and IGPP) can vary year to year based on the projects selected.

The Discovery Park concept is a key component of BNL’s infrastructure renewal plans and continues to make excellent progress. Discovery Park will repurpose approximately 60 acres of federal property at the entrance to BNL to enable joint federal and private development that replaces aging infrastructure and user housing and enables mission enhancing technology transition opportunities. An Alternatives Analysis was completed in FY 2016 and presented to SC. It determined that the most promising approach to achieving the vision for Discovery Park is a mix of federally funded and privately funded development. This approach will construct the proposed SLI-funded SUSC building to provide user and visitor processing and conferencing capability and modern efficient office space to consolidate support staff from non-sustainable WW-II era buildings. This approach will also enable private funding of modern new housing space and other amenities for the thousands of visitors using BNL’s research facilities each year and enable private funding of facilities for technology partnerships compatible with DOE and BNL’s science mission. Work is underway on a model lease to support the initial private facilities to be located adjacent to the SUSC in a dense “user village” concept, now referred to as “Upton Square.” Upton Square will provide the initial development in the overall Discovery Park program with additional research and industry buildings added as they are developed.

The plan for improving asset condition is multipronged and does not solely rely on maintenance investment, which was 1.44% of Replacement Plant Value for 2016. Key to BNL’s strategy is
consolidation out of those assets not worth maintaining, followed by their demolition. Space consolidation will be enabled by renovation and alteration of underutilized buildings and through new proposed buildings, such as the SUSC as part of the Discovery Park development, allowing a major consolidation from inadequate WW-II-era buildings. In addition, there are some proposed GPP projects that would help jumpstart condition improvement efforts for certain critical assets through mission-enabling renovation of key laboratories, and by focusing on utility (water, steam) and facility improvements (roofing, HVAC, and electrical building systems).

The investment strategy relies on the following direct and indirect funding sources:

**DOE SLI funds:** Will be used to perform major building system revitalization or replacement in support of state-of-the-art research facilities that can readily support current and future missions. Over the planning period, BNL has proposed projects to improve the condition of existing buildings and re-task underutilized space that will help to achieve mission needs identified as part of its Site Master Plan process. These proposed projects will revitalize several existing permanent facilities and will be more cost-effective than construction of new facilities and demolition of others.

- **Core Facility Revitalization (CFR) ($74M Preliminary Estimated Budget, FY 2017 proposed start)** involves a preferred option that will re-purpose building 725, a 156,000 sf building constructed in 1981 with additions in 1988 and the 1990s. It contains significant office and high bay space. This project is critical to the ongoing support of the mission need to provide computational and data storage support to current and planned experiments at RHIC and the ATLAS detector at CERN. The space will support the planned growth of computing resources for the RHIC ATLAS Computing Facility (RACF) as well as NSLS-II, CFN, and other Laboratory users. The B725 space will be refurbished for scientific staff currently located in poor space, some of which is WW-II era construction. The extensive underutilized high-bay space supported by the significant power and cooling available, is well suited for conversion to computing use. The scope of the project will potentially include revitalization of the building envelope, HVAC and other building systems, interior finishes, and building configuration as required for performing its new mission. The project received CD-0 in FY 2015; CD-1 was approved in April 2017. The project is proposed to start preliminary design in FY 2017 with a proposed completion in FY 2023.

- **Science and User Support Center (SUSC) ($80M FY 2018 proposed start)** will include construction of a federally funded approximately 100,000 sf office building at the Discovery Park site to enhance user support capability, address major DOE and BNL infrastructure needs, and as an added advantage, to serve as a magnet for further development. This building will enhance operational efficiency by consolidating approximately 300 BNL support division staff, currently dispersed in ten WW-II era substandard buildings, into a single modern office building meeting DOE sustainability goals. In addition to the efficiency gained by collocated staff, the facility’s location at the BNL main entrance will enhance public access for education and commercial outreach for BNL outward facing organizations (such as Procurement and Property Management, the Office of Educational Programs, Technology Commercialization & Partnerships, among others), while supporting BNL core functions. The construction of this building, coupled with the Discovery Park development, will enable footprint reduction leading to demolition of nearly 300,000 sf of WW-II era substandard and inadequate buildings. Full deployment of the Discovery Park vision will also eliminate approximately $27M in deferred maintenance and repair and modernization needs, as resulting vacated buildings are demolished.

- **B911 Renovation for Accelerator Science & Technology ($50M FY 2022 proposed start):** Building 911 is a 106,000 sf building constructed in 1956 with a major addition in 1964. The facility houses the main operations center and staff for the Collider-Accelerator Complex, including RHIC operations. It is expected to be a key facility for eRHIC, if constructed. The revitalization would update most building systems and interior finishes, allowing continued use, with expected completion to support
the start of eRHIC operations.

**GPP (DOE SLI) via the Infrastructure Crosscut:** In response to the initial call for GPP projects that arose out of the FY 2014 Laboratory Operations Board (LOB) Initiative, major recapitalization needs to provide upgraded facilities and infrastructure have been identified and prioritized. These cover several investment types identified by the LOB to address the most urgent gaps including:

- Mission enabling renovations: B801 Hot Cell & Labs
- Facility Improvements: B463 Revitalize Biology Labs; Collider-Accelerator Upgrade HVAC Systems; Collider-Accelerator Upgrade Electrical Distribution Systems; B510 North West Wing Rehabilitate Physics Building; and Replace Roofs Mission Critical Buildings
- Utilities: Site Electrical System Improvements, Site Water System Rehabilitation, Site Steam System Rehabilitation.

**Excess Facilities Disposition (EFD):** In concert with the related infrastructure crosscut call for GPP, BNL has proposed several high impact demolition projects for DOE direct funding. A long-range plan for low impact, lower cost demolitions funded from indirect operating funds has been developed and will be prioritized with other indirect-funded infrastructure needs. EM has committed to incorporating several SC assets into its cleanup program for disposition, but the timeline is uncertain and they may not be accepted by EM until 2030. Included are B491, 650, and 830.

**Indirect Funding:** The Laboratory anticipates increasing overall infrastructure spending over the ten-year period, but also recognizes the possibility that federal budget priorities entering FY 2018 could temporarily alter this approach. These funds include maintenance, including dedicated DMR projects, IGPP, and OIP. OIP projects are not part of the Investment Table but fund alterations, non-capitalized betterment projects, demolition and infrastructure studies. These OIP projects totaled $4.8M in 2016 and are forecast at ~$3.1M in 2017. Collectively, this indirect funding is enabling the execution of the Lab’s space consolidation plans, which when coupled with demolition, will help right-size the BNL footprint, and reduce operations and maintenance costs. Indirect funds are used for non-major recapitalization and sustainment needs using the following strategy:

- Defer major investments in 70+-year-old wood buildings, while performing minimum maintenance to keep these buildings safe and operational. When opportunities arise, consolidate staff from these structures and demolish them.
- Prioritize all proposed investments in infrastructure and ESH and program them to maximize the value of BNL’s infrastructure, reduce risk, and support the Science &Technology programs.
- Begin a program of targeted utility infrastructure investments aimed at revitalizing utilities to meet reliability and capacity needs.

**Non-Federal Funding:** As described previously, BNL is pursuing an innovative public-private partnership concept called Discovery Park as an opportunity to enhance BNL’s DOE mission capability, address infrastructure deficiencies, and contribute to local and regional economic development. The proposed privately funded development of housing and technology partnership facilities would be complementary to the SUSC proposed as an SLI line item project.

Utilization of non-federal funding at BNL has also been demonstrated through a $12.7M Utilities Energy Savings Contract (UESC) project that was completed in May 2015. It included both utilities and building system improvements and in its first full year after implementation achieved 97% of the originally estimated annual energy and green-house gas savings, 88,083 MMBtu and 6,627 MTCO2e respectively. The scope of a second UESC project is being developed for possible implementation in FY 2018 or 2019. Another opportunity that has been explored is a possible combined heat and power project that would provide part of the Lab’s electricity and most of its steam heating requirements at
competitive rates. Current utility rates do not support moving forward with this project, but if energy costs increase in the future, this may become a viable approach.
FERMI NATIONAL ACCELERATOR LABORATORY

Lab-at-a-Glance

Location: Batavia, IL  
Type: Single-program Laboratory  
Contractor: Fermi Research Alliance, LLC  
Site Office: Fermi Site Office  
Website: www.fnal.gov

FY 2016 Costs by Funding Source ($M)

<table>
<thead>
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<th>Category</th>
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<td>NP (NNSA)</td>
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</tr>
</tbody>
</table>

FY 2016 Lab Operating Costs: $417.5 million  
FY 2016 DOE/NNSA Costs: $416.2 million  
FY 2016 SPP (Non-DOE/Non-DHS) Costs: $1.36 million  
FY 2016 SPP as % Total Lab Operating Costs: 0.3%  
FY 2016 DHS Costs: $0 million

Physical Assets:
- 6,800 acres and 366 buildings
- 2.4 million GSF in buildings
- Replacement Plant Value: $2.098B
- 18,849 GSF in 9 Excess Facilities
- 19,771 GSF in Leased Facilities

Human Capital:
- 1,793 Full Time Equivalent Employees (FTEs)
- 8 Joint Faculty
- 85 Postdoctoral Researchers
- 33 Graduate Students
- 55 Undergraduate Students
- 3,245 Facility Users
- 12 Visiting Scientists

Mission Overview

Fermi National Accelerator Laboratory is an international hub for particle physics located 40 miles west of Chicago, Illinois. For 50 years, Fermilab’s employees and users have driven discovery in particle physics by building and operating world-leading accelerator and detector facilities, performing pioneering research with national and global partners, and developing new technologies for science that support U.S. industrial competitiveness. The laboratory’s core capabilities include particle physics; large-scale user facilities and advanced instrumentation; accelerator science and technology; and advanced computer science, visualization, and data. Fermilab’s science strategy for the future delivers on the U.S. particle physics community’s goals as outlined in the Particle Physics Project Prioritization Panel’s 2014 report. The strategy’s primary ten-year goal is a world-leading neutrino science program anchored by the Long-Baseline Neutrino Facility (LBNF) and Deep Underground Neutrino Experiment (DUNE), powered by megawatt beams from an upgraded and modernized accelerator complex. The flagship facility comprised of LBNF and DUNE will be the first international mega-science project based at a Department of Energy national laboratory.

Fermilab’s particle accelerator complex is the only one in the world to produce both low- and high-energy neutrino beams for study. Fermilab integrates U.S. universities and national laboratories into the

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global particle physics enterprise through its Large Hadron Collider (LHC) programs; accelerator science, neutrino science and precision science programs; and dark-energy and dark-matter experiments. Large-scale computing facilities drive research in particle physics and other fields of science. The laboratory’s R&D infrastructure as well as its engineering and technical expertise advance particle accelerator and detector technology for use in science and society. Fermilab’s partnerships and technology transitions programs, including the Illinois Accelerator Research Center, leverage this expertise to apply particle physics technologies to problems of national importance in energy and the environment, national security, and industry.

Fermi Research Alliance, LLC manages Fermilab for the Department of Energy. FRA is an alliance of the University of Chicago and the Universities Research Association, Inc., a consortium of 90 universities. Fermilab’s 6,800-acre site is open to the public every day of the year for recreational activities and self-guided tours.

Core Capabilities

Fermilab has four core capabilities that support the DOE-SC Scientific Discovery and Innovation mission: Particle Physics; Large-Scale User Facilities/Advanced Instrumentation; Accelerator Science and Technology; and Advanced Computer Science, Visualization, and Data.

As the country’s particle physics and accelerator laboratory, Fermilab is the national platform for particle physics and is primarily funded by the DOE Office of High Energy Physics. The laboratory has unique and powerful infrastructure essential to the advancement of discovery in particle physics, including the nation’s only accelerator complex dedicated to particle physics and a suite of particle detectors. Scientific research at Fermilab and around the world is supported by Fermilab’s facilities for design, fabrication, assembly, testing, and operations of particle accelerators and detectors, by its expertise and facilities for computing, and by a talented workforce with globally competitive knowledge, skills, and abilities. The laboratory is thus uniquely positioned to advance the DOE-SC mission in scientific discovery and innovation, with a primary focus on high-energy physics (HEP) and capabilities that address mission needs for advanced scientific computing research (ASCR), particle accelerators for light sources (BES), nuclear physics (NP), and workforce development for teachers and scientists (WDTS).

The laboratory’s four core capabilities are leveraged to deliver on DOE science priorities. High-intensity particle beams are used to answer compelling questions in neutrino science, and reveal new physics phenomena through high-precision tests of the Standard Model of particle physics. High-energy particle beams are used to discover new particles and probe the architecture of the fundamental forces of nature. Underground experiments as well as telescopes are used to uncover the natures of dark matter and dark energy and probe the cosmic microwave background. The 2014 report of the Particle Physics Project Prioritization Panel (P5) identified the long-term science priorities for the U.S. particle physics community, and the laboratory is executing its strategic plan in alignment with DOE and the science community.

1. Particle Physics

Fermilab’s Particle Physics core capability is the heart of the laboratory’s science mission and is defined by four science themes: neutrino science, Large Hadron Collider science, precision science, and cosmic science. Fermilab’s Theory and Theoretical Astrophysics groups perform research at the confluence of these four themes. The laboratory’s accelerators, particle detectors, and fabrication, assembly, testing, and computing facilities provide unique capabilities within DOE and for particle physics research. For example, the Fermilab Test Beam Facility provides test beams for detector R&D and is in high demand for the development of advanced particle detector technologies. The Education and Public Outreach

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FY 2017 Annual Laboratory Plans for the Office of Science National Laboratories
Office and Lederman Science Center support students and faculty in STEM education and support DOE WDTS missions.

**Neutrino science:** Fermilab is the only laboratory in the world that operates two accelerator-based neutrino beams simultaneously, the Neutrinos at the Main Injector (NuMI) beamline and the Booster Neutrino Beamline (BNB). These two intense neutrino sources illuminate an important collection of experiments that are studying neutrinos over both short and long distances, allowing the Fermilab neutrino program to address questions such as whether additional (sterile) neutrinos exist and whether neutrinos violate matter-antimatter (CP) symmetry. The NOvA experiment operates on the high-energy NuMI beamline, and explores the parameters of neutrino flavor transformation. This exploration will become comprehensive with the creation of the Deep Underground Neutrino Experiment (DUNE) in a new beamline created as part of the Long Baseline Neutrino Facility (LBNF). The MicroBooNE experiment on the low-energy BNB searches for sterile neutrinos, and this search will be made comprehensive when the ICARUS detector and Short-Baseline Near Detector (SBND) are both operating in 2019. Experience with these liquid-argon detectors will also inform the future flagship international long-baseline neutrino program, consisting of LBNF and DUNE at Fermilab and in South Dakota. This succession of neutrino experiments is prescribed by the P5 report and will be executed by collaborations of scientists enabled by the capabilities that exist at Fermilab.

**Large Hadron Collider science:** Fermilab serves as the host laboratory for more than 800 university-based U.S. scientists and students working on the Compact Muon Solenoid (CMS) experiment that operates at the Large Hadron Collider (LHC) at CERN, the European center for particle physics. The LHC experiments discovered a Higgs boson in 2012 and have the potential to discover a very broad range of TeV-scale phenomena through both direct and indirect searches. Fermilab is the leading U.S. center for LHC science and second-largest world center after CERN [see 3.2]. In addition, laboratory scientists are engaged in physics analyses of LHC data including studies of the Higgs boson and searches for new phenomena such as supersymmetry, extra dimensions, and dark matter. The laboratory’s globally distributed computational capabilities for the CMS experiment are unparalleled [see 3.4]. Moreover, a skilled and talented workforce of scientists, engineers, and technicians leverages Fermilab’s accelerator and detector R&D programs to contribute essential developments, improvements and upgrades to the CMS detector and the LHC accelerator.

**Precision science:** Fermilab’s precision science theme includes experiments that attempt to reveal gaps in the current understanding of the laws of physics by testing predictions to highest accuracy and searching for phenomena that are either extremely rare or forbidden by current theories. Deviations from expectations are a possible indication of new particles and new interactions. Fermilab has reconfigured accelerator components to create muon beams, and plans to deliver the first such beams to the Muon g-2 experiment in 2017. The beams will increase in intensity over time, culminating with delivery of the world’s most intense muon beams to the Mu2e experiment in 2021. The Muon g-2 experiment will precisely measure a property of muons called the anomalous magnetic moment. Muon g-2 will investigate hints from previous experiments that the muon’s magnetic moment may be different than that predicted by the Standard Model of particle physics. If true, this could be an indication of new physics with far-reaching implications. The Mu2e experiment will search for the spontaneous conversion of muons to electrons. The experiment will be sensitive to new physics manifesting itself in rare processes and corresponding to energies several orders of magnitude higher than those achievable at the LHC, thereby complementing collider experiments’ searches for new particles and new interactions.

**Cosmic science:** Fermilab is a key partner in several world-leading cosmic science experiments, and contributes to R&D efforts toward new dark energy, dark matter, and cosmic microwave background (CMB) experiments. The Dark Energy Survey, whose camera was built by Fermilab and whose science collaboration is led by a Fermilab researcher, ended its fourth year of five years of operations in 2017. Fermilab is working with other DOE laboratories to build new large astrophysical
surveys. The laboratory is engaged in world-leading searches for particle dark matter by operating several first-generation experiments and taking on major responsibilities for the construction of second-generation experiments. Fermilab is a key partner, together with other laboratories, in a CMB research initiative that will establish the world’s best limit on the sum of neutrino masses and help explore the phenomenon of cosmic inflation.

Particle Physics is funded primarily by DOE-HEP with additional funding from DOE-BES (and DOE-SLI for infrastructure), and advances DOE’s Scientific Discovery and Innovation mission (SC 1, 4, 5, 6, 21, 22, 23, 24, 25, 26, 27, 29, 33, 34, and 35).

2. Large-Scale User Facilities/Advanced Instrumentation

Fermilab’s Large-Scale User Facilities/Advanced Instrumentation core capability encompasses two DOE-SC user facilities: the Fermilab Accelerator Complex and the CMS Center, which together supported more than 3,200 users in FY16. The laboratory has the human capital and infrastructure essential to developing, designing, constructing, and operating large-scale user facilities.

**Fermilab Accelerator Complex**: The Fermilab Accelerator Complex is the nation’s only accelerator complex dedicated to particle physics, and the second largest particle physics accelerator complex in the world after CERN. Research at this user facility has led to many discoveries over more than 40 years of operation, including the top quark, bottom quark, tau neutrino, determination of the properties of charm- and bottom-quark systems, and numerous precision measurements such as the discovery of new matter-antimatter asymmetries in kaon decays and the world’s best determination of the mass of the W boson.

The Fermilab Accelerator Complex comprises seven particle accelerators and storage rings with particle-beam capabilities found nowhere else in the world. Fermilab uniquely supplies two very intense neutrino sources (the low-energy Booster neutrino beam and the high-energy NuMI beam) that enable the physics programs of the NOvA, MicroBooNE, and MINERvA experiments. By 2019 the Booster neutrino beam will deliver neutrinos to a new three-detector short-baseline neutrino program. The Fermilab Test Beam Facility is the only location in the United States that enables detector R&D tests with high-energy hadron beams, and is used by more than 200 international researchers annually. Reconfiguration and upgrades of the accelerator complex will turn Fermilab into the world center for the study of muons by delivering high-intensity muon beams to the Muon g-2 and Mu2e experiments. Future upgrades of the accelerator complex will provide megawatts of beam power to the Long-Baseline Neutrino Facility (LBNF) and Deep Underground Neutrino Experiment (DUNE).

**CMS Center**: For almost two decades Fermilab has served as the host laboratory for the more than 800 scientists and students from about 50 U.S. universities who work on the CMS experiment at the LHC. Researchers using Fermilab’s CMS facilities played leading roles in the 2012 Higgs boson discovery, and ongoing research promises to further revolutionize our understanding of the universe.

The CMS Center consists of the LHC Physics Center (LPC), CMS Remote Operations Center, and the U.S. CMS Computing Facility at Fermilab. The LPC is designed to engage members of U.S. CMS institutions distributed across the country in physics analyses of LHC data and CMS detector upgrades. The LPC achieves this by lowering the barrier to remote participation and creating a thriving environment for collaboration among participating institutions. Through the Distinguished Researcher and guest and visitor programs, collaborators are supported to spend significant time resident at the LPC, while the CMS Data Analysis School draws 100 participants each year. The Remote Operations Center enables physicist participation in remote operations and monitoring of the CMS detector, and keeps scientists, students, and technicians connected to operations activities at CERN. The U.S. CMS Computing Facility at Fermilab is the largest and most reliable computing Tier-1 facility worldwide (after the CERN Tier-0 center). As part of a worldwide grid computing capability this facility is available to qualified CMS.
researchers around the world. Fermilab has proposed to make the CMS Center a national user facility, and this proposal is currently under review.

**Advanced Instrumentation:** An experienced and talented workforce at Fermilab conceives and develops state-of-the-art particle detector technologies and uses them to construct detector systems. Achievements include the development of very-low-mass silicon detectors for particle physics collider experiments, CCD detectors for the Dark Energy Camera, scintillator detectors used for a wide variety of particle physics experiments, and Liquid Argon Time Projection Chambers (LArTPCs) used by current neutrino experiments and the future flagship experiment, DUNE. Fermilab's advanced instrumentation capability is used to develop and construct upgrades for the CMS detector at the Large Hadron Collider, including innovative silicon trackers, a silicon-based calorimeter, readout electronics, and R&D for precision timing detectors.

*Large-Scale User Facilities/Advanced Instrumentation is funded primarily by DOE-HEP (and DOE-SLI for infrastructure), and advances DOE's Scientific Discovery and Innovation mission (SC 1, 4, 5, 6, 21, 22, 23, 24, 25, 26, 27, 29, 33, 34, and 35).*

3. Accelerator Science and Technology

Fermilab’s Accelerator Science and Technology core capability includes five core competencies, strategically aligned with recommendations of the 2015 HEPAP Accelerator R&D sub-panel: high-intensity particle beams; high-power beam targets; high-field superconducting magnets; high-gradient and high-quality-factor superconducting radio-frequency (RF) cavities; and accelerator science and technology training. These core competencies are enabled by unique accelerator and beam test facilities and world-leading expertise that sustains Fermilab’s strategic goal to maintain its world leadership in high-intensity and high-energy accelerator applications. Fermilab has established strategic partnerships in accelerator science and technology with leading universities including Northern Illinois University, Illinois Institute of Technology, Northwestern University, Cornell University, and the University of Chicago. Fermilab’s Illinois Accelerator Research Center is uniquely positioned to cement partnerships with industry and universities to increase strategic partnership projects and to advance DOE’s accelerator stewardship program.

**High-intensity particle beams:** Fermilab operates the world’s most advanced high-intensity proton accelerator complex dedicated to particle physics. The ongoing Proton Improvement Plan (PIP) and a subsequent upgrade project (PIP-II) will maintain Fermilab’s international leadership and support the next generation of neutrino and precision science experiments. PIP-II leverages laboratory capabilities in accelerating and transporting high-intensity beams in circular and linear accelerators, and is needed as the next step to achieving a beam power of 2.4 MW. Results from accelerator R&D at Fermilab support the flagship neutrino science program and influence how U.S. and international accelerators are designed, constructed, and operated. Fermilab has achieved more than 700 kW beam power to the NOvA experiment and is running around 2x10^17 protons per hour from the proton source to support the short baseline neutrino and muon experiments.

**High-power beam targets:** Beam targets are currently limited to beam powers of 1 MW. Fermilab is developing beam target technologies to address the challenges of design, construction, and operation of multi-MW target facilities. The laboratory is leading the collaborative R&D effort on new radiation- and thermal-shock-compatible materials and technologies.

**High-field superconducting magnets:** Fermilab has a long history of developing, fabricating, and delivering advanced superconducting magnets, such as the world’s first superconducting dipole magnets deployed in a circular collider (the Tevatron). The laboratory’s core competency in high-field superconducting magnets, including novel magnetic materials and electromechanical magnetic design, is essential to the luminosity upgrades of CERN’s LHC accelerator. This core competency is also critical to
enable upgrades of the LHC for operations at higher energies, which would require further increases in the maximum magnetic field achievable in accelerator-quality magnets. Infrastructure supporting Fermilab’s magnet work includes superconducting strand and cable testing equipment, cable making, coil winding machines, collaring presses, reaction ovens, a cryogenic vertical magnet test facility for cold masses, a cryogenic horizontal magnet test facility for magnets in cryostats, and cryogenic infrastructure.

**High-gradient and high-quality-factor SRF cavities:** Fermilab’s SRF expertise and infrastructure comprise a globally renowned core competency in the fabrication and testing of SRF technology. Laboratory staff members play an important role in the design and planning of linear and circular accelerators around the world that depend on SRF technology. This core competency enables Fermilab to be a key partner in the construction of the superconducting linear accelerator for SLAC’s LCLS-II free electron laser, the highest-priority construction project in the DOE Office of Science. Fermilab’s experienced staff and extensive infrastructure led the way in the design of SRF cryomodules and cryogenic infrastructure for LCLS-II, and extended the state of the art for SRF cavity performance. By working with SLAC National Accelerator Laboratory and Thomas Jefferson National Accelerator Laboratory to establish LCLS-II as a world-leading facility, Fermilab is contributing its unique infrastructure and expertise to the broader scientific endeavor while simultaneously enhancing in-house capabilities for future projects such as PIP-II. This infrastructure and expertise also positions the laboratory to contribute to potential future accelerators and colliders. SRF infrastructure includes chemical processing and high-pressure rinsing of cavities, processing and brazing furnaces, cleanroom assembly facilities, inspection and testing capabilities for both bare and dressed cavities, cryomodule assembly stations, and a complete cryomodule test facility.

**Beam test facilities:** The Fermilab Accelerator Science and Technology (FAST) facility hosts a unique program of advanced accelerator R&D at the Integrable Optics Test Accelerator (IOTA) ring. The research promises to advance accelerator science and enable high-intensity accelerator technologies for multi-megawatt proton beams. An electron injector to the IOTA ring provides an additional platform for accelerator science and technology.

**Accelerator science and technology training:** Fermilab is making significant contributions to the nation’s accelerator science and technology workforce training. The laboratory hosts the United States Particle Accelerator School (USPAS), which has trained over 4500 students since its inception in 1981 and has recently undergone a restructuring that re-establishes the USPAS as a Fermilab program. Fermilab also maintains a renowned joint university/laboratory doctoral program in accelerator physics and technology, as well as several undergraduate summer internship programs in collaboration with Argonne National Laboratory.

*Accelerator Science is funded by DOE-HEP with additional funding from DOE-BES (and DOE-SLI for infrastructure), and advances DOE’s Scientific Discovery and Innovation mission (SC 1, 4, 21, 22, 24, 25, 26, 33, 34, and 35).*

### 4. Advanced Computer Science, Visualization, and Data

Fermilab’s expertise in Advanced Computer Science, Visualization, and Data enables scientific discovery. This core capability complements theory and experiment to increase scientific knowledge through data collection, storage, reconstruction, and analysis, as well as through scientific simulations. Fermilab has a remarkable history of developing, delivering, and deploying computing technologies for the scientific community.

Fermilab scientists and engineers are internationally recognized as experts in high-performance computing algorithms, scientific workflow systems and analysis frameworks, sophisticated scientific simulations, and data analytics toolkits. A prominent and successful example is a community software
framework and scientific workflow engine (the “art” framework) that is being adopted by the U.S.-based neutrino and muon experimental communities and by some of the direct-detection dark matter experiments.

Fermilab is recognized for expertise in designing, developing, and operating distributed computing infrastructures and facilities, petascale scientific data management, and scientific workflows for data recording, processing, and analysis. The laboratory provides access to large-scale computational and data-management facilities for the CMS experiment at CERN, the LHC Physics Center, neutrino science and precision science experiments, the Dark Energy Survey, computational cosmology, lattice QCD, and accelerator simulations.

The laboratory is a leader in grid computing, which originally evolved to satisfy the rapidly expanding data needs of LHC experiments and is now in use by other areas of science, industry, government, and commerce. Fermilab scientific computing facilities use grid technology to share resources for data processing, storage, and analysis. Fermilab is a leader in providing grid computing resources to scientific organizations outside DOE-HEP through the Open Science Grid, a consortium dedicated to providing secure access to distributed high-throughput computing for scientific research in the U.S. The newly developed HEPCloud capabilities enable Fermilab to provide to its users access to commercial cloud resources and ASCR HPC resources. Experiments such as CMS, Mu2e and NOvA are already starting to exploit Fermilab’s HEPCloud capabilities.

Due to the collaborative nature of particle physics research, Fermilab does not develop scientific software or computing capabilities in isolation. The laboratory has formed partnerships with all the DOE Office of Science laboratories as well as international laboratories (such as the European laboratory CERN, DESY in Germany, and KISTI, the Korean Institute of Science and Technology Information) to work on projects that include the Open Science Grid, accelerator modeling, computational cosmology, and particle physics simulations. Fermilab’s strategy is to leverage ASCR expertise where appropriate to respond to computational challenges presented by the DOE-HEP program through the judicial use of partnership programs such as DOE’s Scientific Discovery through Advance Computing (SciDAC) program, as well as periodic ASCR calls for proposals.

Fermilab’s data center is the single largest U.S. HEP computing center with 80,000 processing cores, 30 petabytes of disk storage, and nearly an exabyte of data storage on robotic tape systems. State-of-the-art computational facilities enable the laboratory to develop new capabilities to support the scientific missions of Fermilab and DOE. Fermilab plays an essential role in developing software and hosting scientific computing projects and three major computing facilities for the science community: a CMS Tier-1 Center, Lattice QCD Computing, and FermiGrid.

**CMS Tier-1 Center**: The CMS experiment uses a distributed computing model in which data distribution, processing and delivery is handled by seven international Tier-1 centers together with university- and laboratory-based Tier-2 computing and storage facilities. This computing model satisfies the needs of particle physicists by providing data storage and processing power on an extreme scale, interconnected by the strongest networks. The CMS Tier-1 Center at Fermilab is the most powerful worldwide (after CERN’s Tier-0 center) for the 3,000-member, 41-country CMS experiment.

**Lattice QCD Computing**: Quantum chromodynamics (QCD) is the theory that describes how quarks and gluons interact via the strong force and predicts the properties of hadrons such as the proton, neutron, and pion. QCD calculations involve numerical simulations performed on a lattice of space-time points (known as Lattice QCD) that can be extremely computationally intensive. Fermilab builds and operates large computer clusters for such calculations as part of DOE’s national Lattice QCD computational infrastructure. Fermilab scientists and engineers also participate in a DOE SciDAC-2 program devoted to the improvement of software for Lattice QCD computing.
FermiGrid: Fermilab is the host laboratory for several neutrino and precision science experiments and provides computing facilities for these experiments, including reliable resources for data recording and processing (the equivalent of the CERN LHC “Tier 0” for neutrino and precision science). FermiGrid is the primary HEP facility for non-LHC computing and provides computing and storage resources that are shared among these experiments.

Advanced Computer Science, Visualization, and Data is funded primarily by DOE-HEP with additional funding from DOE-ASCR (and DOE-SLI for infrastructure), and advances DOE’s Scientific Discovery and Innovation mission (SC 1, 4, 5, 6, 21, 22, 23, 24, 25, 26, 27, 29, 33, 34, and 35).

Science Strategy for the Future

Fermilab’s science strategy for the future has as its primary ten-year goal a world-leading neutrino science program powered by megawatt beams from an upgraded and modernized accelerator complex. This national flagship particle physics initiative comprises the Long-Baseline Neutrino Facility (LBNF) and the Deep Underground Neutrino Experiment (DUNE). LBNF/DUNE will be the first-ever large-scale international science facility hosted by the United States. Identified by the U.S. particle physics community in its consensus P5 report as the highest-priority domestic construction project in its timeframe, LBNF/DUNE is attracting global partners willing to invest significant financial, technical, and scientific resources. A five-year program that includes current and near-term neutrino experiments and an R&D platform that serves the wider neutrino physics community is driving the development of capabilities and bringing together the international community needed for LBNF/DUNE.

Fermilab’s success in operating intense low- and high-energy neutrino beams, its core scientific and technical capabilities, its project management expertise, and its international reputation as an excellent scientific partner are making it the destination of choice for the world’s neutrino researchers.

Artist's rendering of the Long-Baseline Neutrino Facility (LBNF) that will send a very intense beam of neutrinos 800 miles to a massive liquid-argon detector located deep underground in the Sanford Underground Research Facility in South Dakota.

As the country’s particle physics and accelerator laboratory, Fermilab is moving forward with new experiments, new international and national partnerships, and R&D programs that support all of the science drivers identified in the P5 report. Over the next decade Fermilab will continue to be the leading U.S. center – and the second leading center in the world - for Large Hadron Collider science, enabling leading roles for U.S. scientists in future LHC discoveries and driving key contributions to upgrades of the LHC accelerator and the CMS detector. The start of the Muon g-2 and Mu2e experiments will turn Fermilab into the world center for the study of muons, particles whose properties may open a window onto new physics. Fermilab will support the community-endorsed diversified approach to dark
matter detection, including key roles in the Generation 2 dark matter projects. The laboratory’s leading role in the Dark Energy Survey, supporting roles in its successor experiments, and involvement with the South Pole Telescope will ensure continued U.S. leadership in the study of cosmic acceleration. In partnership with academics from nearby universities and colleagues at the Argonne National Laboratory, Fermilab will establish Illinois as a world center for advanced accelerator research with a suite of unique test facilities and R&D programs that will drive major advances in accelerator science and technology.

Fermilab’s core capabilities define the scope of the laboratory’s science and technology strategy. Major initiatives in people, infrastructure and R&D support the strategy. The laboratory will devote the majority of its time and effort over the next ten years to major initiatives identified for each of the four core capabilities. Major initiatives are presented in the following sections.

Infrastructure

Overview of Site Facilities and Infrastructure

The Fermilab Campus Master Plan\(^3\) supports the implementation of the P5 plan for U.S. particle physics and Fermilab’s strategic plan. The master plan is the cornerstone for mission-based facility planning at the laboratory, and it guides the actions of the Campus and Facility Planning Board that ensures coordination, communication, and prioritization for facilities projects. The master plan encompasses three design themes: modernization of facilities; consolidation and centralization of dispersed and inefficient support facilities; and preservation of the laboratory’s unique character and identity. Urgent needs to centralize, consolidate, and modernize scientific, technical, and engineering facilities will begin to be solved by the Integrated Engineering Research Center (IERC) [see 4.5]. The Science Laboratory Infrastructure (SLI) funded Utilities Upgrade Project is nearing completion and represents the types of investment needed for modernization of utilities across the site. The SLI-funded Wilson Hall revitalization project, which received full funding of $9M SLI GPP in FY 2016, will greatly improve efficiencies and density in the lab’s largest administrative building and enhance circulation for collaboration within the IERC.

Operating the Fermilab site for science requires the use of buildings, real property trailers, and tunnels as well as hundreds of miles of utility infrastructure including roads, electrical, natural gas, potable water, and sanitary systems. A one-of-a-kind utility system consisting of miles of underground supply pipe, five pumping stations, miles of return ditches, and 80 acres of surface water ponds enables industrial cooling water to also be used for fire protection. The total real property Replacement Plant Value (RPV) is $1.037B, excluding the laboratory’s programmatic accelerator and tunnel assets. Property information associated with all assets is maintained in the DOE’s Facilities Information Management System (FIMS) real property database, and is available on site through the Fermilab Infrastructure Database and Geographic Information System. A summary of physical assets is included in Section 2 (Lab-at-a-Glance). All of the laboratory’s real property is used and owned by DOE. Property usage is predominately divided among research and development space and administrative areas. Unoccupied land is maintained as restored prairie, tilled agriculture, or woodland and is preserved for future science needs.

Executing the master plan and continuing a demolition program will reduce the number of buildings, trailers, and overall gross square footage. In FY 2016, the demolition of the Master Substation and two Main Ring service buildings totaling 6,482 gross square feet was completed using overhead funds. The goal for FY 2017 is to complete the demolition of the Site 39 trailer, the Industrial Center Building.

\(^3\) http://fess.fnal.gov/master_plan/index.html
trailers, and the Main Ring Gazebo, totaling 11,497 gross square feet. During FY 2016, Fermilab added
one building and one entry under Other Structures and Facilities (OSF) to the FIMS inventory.

Table 4 summarizes the number of facilities and gross square footage for different types of facilities and
their conditions.

Table 1. Types and Conditions of Facilities

<table>
<thead>
<tr>
<th>Types of Facilities</th>
<th>Number of Facilities</th>
<th>Gross Square Footage of Facilities</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Adequate</td>
<td>Substandard</td>
</tr>
<tr>
<td>Other Structures and Facilities</td>
<td>46</td>
<td>1</td>
</tr>
<tr>
<td>Mission Unique Facilities</td>
<td>99</td>
<td>0</td>
</tr>
<tr>
<td>Non-mission Unique Facilities</td>
<td>216</td>
<td>34</td>
</tr>
</tbody>
</table>

Fermilab completed the Laboratory Operations Board (LOB) infrastructure assessment in FY 2014, which
provided an opportunity to extend the effort that began with the development of the Campus Master
Plan by working with users and scientists to validate the results of the plan and establish the campus
strategy. Electrical substations and the industrial cooling water piping system are two “Other Structures
and Facilities” assets that were rated as substandard during the initial LOB assessment but have since
been improved through the SLI Utility Upgrade Project. Lab space accounts for 46% of the substandard
and inadequate non-mission unique facility square footage, and two-thirds of the lab space is in light
industrial-frame buildings constructed in the Fermilab Village shortly after the laboratory was founded.
The remaining 54% consists of real property trailers or residential houses constructed before the
Fermilab land acquisition and is used for housing, office and storage space.

In non-excess facilities with overall utilization less than 75%, there are 173,861 gross square feet
identified as underutilized in FIMS, based on the space type utilization level. This includes space with
utilization ranging from 0% to 70% within those facilities.

There are nine assets currently identified as excess facilities in FIMS, totaling 18,849 gross square feet.
While these facilities are planned for near-term demolition, they are still occupied and in use.
Accordingly, the FY 2016 carrying costs for these facilities included annual actual maintenance and
operating costs totaling $80,589. The nine assets include the Lab 8 House, one D0 trailer and seven
Industrial Center Building trailers. A pilot project to demolish two accelerator service buildings around
the Main Ring while preserving utilities necessary to serve underground experimental areas has been
completed. Now that the pilot project is complete, it is expected that an additional 36 accelerator
service buildings will be added to the excess facilities list and scheduled for demolition in the future. As
part of the April 2015 LOB Excess Facilities Working Group request, Fermilab has identified 55 additional
buildings for future excess, including the accelerator service buildings, Village lab buildings, and office
trailers. Demolition of the accelerator service buildings is complicated, due to infrastructure
requirements of future projects. Demolition estimates have been refined based on the pilot project.
Excess characterization and priority data for these assets has been populated in FIMS, concurrent with
submittal of the Annual Laboratory Plan. Full implementation of the master plan will relocate additional
functions and personnel from geographically remote locations to the central and technical campuses, thereby vacating legacy facilities that will also be slated for demolition.

**Campus Strategy**

Fermilab’s campus strategy implements the Campus Master Plan, thus enabling the laboratory to deliver on the U.S. particle physics community’s science goals as outlined in the P5 plan. In addition to reducing inefficiencies associated with functional obsolescence and geographically dispersed facilities, the campus strategy represents a comprehensive approach to Fermilab’s future infrastructure.

The campus strategy has four primary objectives:

- Construct sustainable infrastructure that will attract international investment and the brightest minds to the world’s leading laboratory for accelerator-based neutrino science.
- Maximize productivity by establishing an atmosphere of “eat-sleep-work to drive discovery” that efficiently meets the needs of the scientific community.
- Integrate into one geographic area the entire life cycle of research, engineering, fabrication, and operations expertise for accelerators and detectors.
- Consolidate, centralize, and modernize to optimize operational resources, maximize efficiency, enhance communication, and foster succession planning.

These objectives address the needs of the laboratory’s core capabilities by providing facilities and infrastructure to close identified infrastructure gaps that include:

- Sufficient space for project teams and international users for the first-ever large-scale international science facility hosted in the United States.
- Buildings nearer where the work is for efficient matrixed resources for projects and operations.
- Increased high-bay space for production facilities.
- Modernized facilities with modular walls and furniture for efficient reconfiguration.
- Short-term accommodations for a growing number of collaborating visitors and users.
- State-of-the-art computing facilities.

Table 5 provides a roadmap for planned investments in specific projects that are needed to close these gaps.

The laboratory’s utility infrastructure will also continue to require further investment to accommodate ongoing operations and future mission needs. The SLI-funded Utility Upgrade Project that is nearing completion will eliminate the lab’s largest vulnerabilities.

When siting future projects, Fermilab’s Facilities Engineering Services Section works closely with the Chief Research Officer, experimental planning groups, project teams, the laboratory’s Campus and Facility Planning Board, and the Office of Campus Strategy and Readiness to efficiently use existing facilities or develop plans to expand facilities. Infrastructure gaps are prioritized according to mission need.

The IERC remains the highest-priority project needed to bring the technical and scientific resources that are currently scattered across the site into closer proximity to foster a more effective and efficient work environment. The IERC is expected to support other Office of Science programs in addition to Fermilab’s core Office of High Energy Physics programs. For technical and scientific personnel who will have both project and operational responsibilities, the IERC will enable them to perform both functions more effectively and shift more easily between activities. The resulting productivity improvements will be necessary for success in an era when Fermilab is carrying out a large project portfolio. IERC has obtained
CD-1 and anticipates Project Engineering and Design (PED) funding in the next budget. IERC begins to satisfy the most urgent needs to relocate resources to the Central Campus in accordance with priorities established by the P5 plan.

In the 2015 annual update to the Fermilab Campus Master Plan, an assessment was carried out of future directions in international accelerator collaborations, both for operation of current accelerators and construction of new machines. The result was the creation of the Global Accelerator Center project that is proposed to do for scientists what the IERC does for engineers. The Global Accelerator Center will be located in the central campus just south of Wilson Hall and the IERC.

Fermilab site map. Buildings are highlighted in orange. The Fermilab Village, which is located on the east side of the site (shown on the right side of the map), includes both residential and technical legacy facilities. Functions housed in the technical facilities will be relocated to the central (A) and technical (B) campus areas.
The master plan defines a Central Campus that is centered on Wilson Hall and includes a new scientific hostel (guesthouse) that fulfills the “sleep” portion of the “eat-sleep-work to drive discovery” theme. The hostel will meet the growing needs of short-term visitors, thereby supplementing the longer-term housing in the Fermilab Village. A schematic design and preliminary site selection has been completed. The next step in the planning process includes an alternatives analysis to determine funding options with possible business models. The Central Campus also includes the future sites of the PIP-II and PIP-III accelerator upgrade projects, which provide the beam power needed to support the laboratory’s future world-leading program in neutrino science, and developing site plans for an envisioned upgrade to support infrastructure and next generation accelerator technology.

The laboratory has started the first step of the Wilson Hall 2.0 modernization that began in FY 2016 with $9M from SLI’s GPP program. This project increases density through standardized floor plans and begins to implement a standard for reconfigurable walls and furniture. Additionally, this project will help the connectivity with the adjacent IERC. Other GPP crosscut candidates in the Central Campus are the Central Utility Building improvements and Excess Facilities Removal projects.

Just south of the Central Campus is the Muon Campus. Fermilab is nearing completion of construction of the Muon Campus activities. Significant investment through the DOE Office of High Energy Physics (DOE-HEP) has allowed the redevelopment and repurposing of existing infrastructure in support of the Mu2e and Muon g-2 science projects. Within a short walking distance from the Central Campus is the Neutrino Campus, hosting the Liquid Argon Test Facility that houses the MicroBooNE detector, and the Short-Baseline Neutrino (SBN) program. Construction of two new general-purpose detector hall buildings for the SBN program is nearing completion.

The Technical Campus houses fabrication, production, and testing facilities for LCLS-II and PIP-II cryomodules, high-field magnets for CERN’s LHC accelerator, and solenoids for Mu2e. The challenge for the Technical Campus is to provide the needed capability for production capacity given the availability of limited production space. The first step towards satisfying this infrastructure gap is to construct the Industrial Center High Bay Addition. Initially proposed as a possible SLI project, further definition of the requirements and a more urgent timeframe have resulted in a change in strategy to meet the need using DOE-HEP GPP funding in FY 2017 and FY 2018. Design of this new facility is underway with construction start expected in FY 2018.
Deferred maintenance requirements and projections are shown in Table 6. Of the deferred maintenance identified for FY 2016, the laboratory’s utility infrastructure, shown as “Other Structures and Facilities” (OSF) in Table 4, currently comprise 76% of the site’s total FY 2016 deferred maintenance backlog, or $30M of a total $39M. It is important to note that the SLI Utility Upgrade Project that is nearing completion reduced deferred maintenance at the end of FY 2016 by $8.3M. The integrated facilities and infrastructure cross-cut budget profile through FY 2020 includes investments in domestic water and industrial cooling piping systems, the Central Utility Building and computing upgrades, and support for the Short-Baseline Neutrino program [see Table 5]. While additional utility GPP projects are identified in the lab’s five-year infrastructure budget plan, the investment via the Office of Science’s SLI Modernization Initiative proved critical for improved utility reliability for existing and future science needs. The combination of ongoing maintenance at 2% of Fermilab’s conventional replacement plant value, laboratory and Office of Science GPP projects, SLI investment, and substantial demolition of facilities is expected to control the deferred maintenance backlog to an acceptable level.

Fermilab’s core capabilities are subject to the same risks described above from deferred maintenance and infrastructure gaps. Previously, the highest infrastructure risk was a potential failure of Fermilab’s Master Substation. This risk is now mitigated with the SLI UUP nearing completion and the new MSS fully operational. The second risk is the continued inefficiency in operations, particularly in terms of functionally obsolete buildings, geographically dispersed locations, utility failures due to aging systems, isolated downtimes due to localized failures, and resources consumed by excess facilities. Several legacy buildings from the original site development in the Fermilab Village are still used for lab space and manufacturing facilities despite being classified as inadequate or substandard under the LOB assessment. A candidate for an FY 2019 GPP crosscut is funding for Excess Facilities Removal of these and other buildings as elements of the Campus Master Plan are implemented and such functions are relocated to modern facilities in the Central Campus.
Lab-at-a-Glance

**Location:** Berkeley, CA  
**Type:** Multi-program Laboratory  
**Contractor:** University of California  
**Site Office:** Berkeley Site Office  
**Website:** [www.lbl.gov](http://www.lbl.gov)

**Physical Assets:**
- 202 acres and 94 buildings
- 1.68 million GSF in buildings
- Replacement Plant Value: $1.335B
- 410 GSF in 1 Excess Facility
- 326k GSF in Leased Facilities

**Human Capital:**
- 3,302 Full Time Equivalent Employees (FTEs)
- 232 Joint Faculty
- 486 Postdoctoral Researchers
- 263 Graduate Students
- 148 Undergraduate Students
- 11,403 Facility Users
- 2,241 Visiting Scientists

**FY 2016 Costs by Funding Source ($M):**
- BER $147
- BES $160
- ASCR $140
- HEP $82
- SPP $100
- DHS $5
- Other DOE $24
- Other SC $13
- NP $23
- EERE $77
- EM $10
- NE $3
- NNSA $17
- Other DOE $24
- NNSA $17
- Other SC $13
- NP $23
- EERE $77
- EM $10
- NE $3
- NNSA $17

**Mission Overview**

Established in 1931, Lawrence Berkeley National Laboratory (Berkeley Lab) plays an important and distinctive role within DOE’s network of great national laboratories. From discovery science to mission-driven basic research, Berkeley Lab develops science and technology solutions for the benefit of the nation and the world.

Berkeley Lab specializes in integrative science and technology, leveraging our world-renowned expertise in materials, chemistry, physics, biology, environmental science, mathematics, and computing to conduct forefront research. We advance the frontiers of science and technology through three approaches: advanced instruments and user facilities, large team science, and research programs led by one or a few outstanding investigators. These three approaches are closely integrated to the benefit of the entire research program.

The mission of Berkeley Lab, to bring science solutions to the world, runs deep within the organization. Our five national user facilities serve over 11,000 researchers every year, one third of all the national lab network users. We collaborate closely with other national laboratories on projects from high energy and nuclear physics to subsurface science, exascale computing, and plant genomics. Finally, the Lab’s Energy
Sciences network (ESnet) provides the powerful data connectivity needed for the system of national laboratories to operate as a network of discovery.

Berkeley Lab’s close relationship with the University of California brings the intellectual capital of the university’s faculty, postdocs and students to bear on the pursuit of DOE’s science and energy missions. The Lab’s scientific strength is enhanced by its open programs and culture, its integrative science and technology, and its emphasis on collaboration with the national and global scientific community – sharing our world class user facilities, research and expertise to solve the challenges that define our time.

Core Capabilities

Each of Berkeley Lab’s Core Capabilities involves a substantial combination of people, facilities and equipment to provide a unique or world-leading scientific ability to support DOE missions and national needs. Each is executed safely, with minimal impact on the environment and surrounding community. The descriptions below summarize Berkeley Lab’s Core Capabilities, their targeted missions and their funding sources.

The Core Capabilities lend an exceptional depth to Berkeley Lab’s broad research portfolio while enabling an integration of efforts to better support the DOE missions. To emphasize their strategic nature, the Lab has grouped these Core Capabilities into scientific themes: Large Scale User Facilities/Advanced Instrumentation; Basic Research in Energy; Biological and Environmental Sciences; Computing and Mathematics; High Energy and Nuclear Physics; Accelerator Science and Technology; and Applied Science and Energy Technology.

1. Large Scale User Facilities/Advanced Instrumentation

Since its inception as the first accelerator laboratory, Berkeley Lab has had an overarching Core Capability of designing, constructing and operating leading scientific facilities for large user communities. Among the national lab system, Berkeley Lab has the largest population of users, who produce scientific breakthroughs because of their creative work at these facilities. Below are summary descriptions of the Laboratory’s large-scale user facilities. Core Capabilities in other sections of this report, such as Basic Research in Energy, Computing and Mathematical Sciences, and Applied Science and Energy Technology, are key to the success of Berkeley Lab’s advanced facilities and instrumentation.

The Advanced Light Source (ALS) is the world-leading facility for high-brightness soft X-ray science, with additional excellent performance in the hard X-ray and infrared spectral regions. ALS researchers use the data they collect to understand, predict and ultimately control the flow of matter and energy at length scales ranging from the atomic to the macroscopic. This research underpins many of DOE’s Core Capability areas, including those involving chemical, material and biological systems. In 2016, this facility supported the research of 2,317 scientist users, and ALS-based results appeared in 977 refereed journal articles. Funded primarily by BES, it has an annual budget of ~$60 million.

The Molecular Foundry provides users with expert staff and leading edge instrumentation for multidisciplinary, collaborative nanoscale research. Users come from academic, industrial and national laboratories, from within the U.S. and abroad. For FY16, research at the Foundry resulted in 344 publications. The Molecular Foundry encompasses facilities specializing in characterization, made up of the National Center for Electron Microscopy, along with Imaging and Manipulation of Nanostructures facility; Nanofabrication; Theory of Nanostructured Materials; and synthesis, focusing on Inorganic Nanostructures, Biological Nanostructures; and Organic and Macromolecular Synthesis. The Foundry’s FY16 BES budget was $27.6 million, with 774 onsite and remote users.
The **DOE Joint Genome Institute (JGI)** is a national user facility carrying out projects of central relevance to DOE missions in alternative energy, global carbon cycling and biogeochemistry. JGI is the world’s largest producer of plant and microbial genomes, with programs focused in three areas: large-scale generation of DNA sequences, development of innovative DNA analysis algorithms, and a strategic focus on functional genomics that includes a growing DNA design and synthesis program. It has more than 1,350 users per year; its FY17 budget of ~$69 million is funded primarily by BER. Berkeley Lab recently completed an extensive international search for the JGI Director and selected Nigel Mouncey to lead the JGI beginning March 15, 2017. Dr. Mouncey formerly served as Research and Development Director for Bioengineering and Bioprocessing at DOE AgroSciences LLC, and brings more than 18 years of experience in the industrial biotechnology industry in strategic, technical and management positions.

The **National Energy Research Scientific Computing Center (NERSC)** is the high performance scientific computing facility for the DOE’s Office of Science. NERSC supports more than 6,000 users from universities, national laboratories and industry, representing the largest and most diverse research community of any DOE user facility. NERSC is the principal provider of high performance computing services to SC’s six scientific programs. NERSC’s resources include large-scale, state-of-the-art computing and data systems, networking, and expert consulting and support services. In 2016, NERSC completed the installation of the “Cori” supercomputer. A hybrid system, with both “traditional” Intel Xeon processors and energy-efficient Intel Xeon Phi manycore processors, Cori sets the SC user community on the path to exascale. With most of its computing capability residing in the Xeon Phi processors, Cori’s peak performance is about 30 petaflops; the system was ranked the world’s fifth most powerful supercomputer on the November 2016 Top 500 list. In addition to its raw computational capability, Cori has special features to support the growing data intensive SC workload, including a layer of solid-state flash storage that serves to accelerate application I/O performance. NERSC’s scientific impact is enormous: more than 1,900 scientific publications cite NERSC each year. In 2017 alone, its current systems, Cori (NERSC 8) and Edison (NERSC-7), will provide on the order of six billion computational hours to researchers. The NERSC Division also manages the data-analysis systems for the JGI and the high-energy and nuclear physics groups at Berkeley Lab. NERSC’s FY16 funding was $84 million, provided by ASCR.

The **Energy Sciences Network (ESnet)** is the mission network of the DOE, a dedicated high-performance network infrastructure optimized for very large scientific data flows. ESnet provides connectivity for all major DOE sites and facilities, and joins them to more than 150 research and commercial networks around the world. Every day, tens of thousands of DOE-funded researchers at national laboratories and in universities depend on ESnet’s infrastructure, and the network transports roughly 50-60 petabytes of science data each month. During FY16, ESnet started ESnet6, a strategic facility project to upgrade its network to meet the needs of exascale computing. In addition, ESnet is revamping its requirements review process across the SC program offices. ESnet’s FY16 funding is ~$38 million (ASCR), with a total of 61 users and 17 facility publications.

**Basic Research in Energy**

**2. Chemical and Molecular Science.**

Berkeley Lab has world-leading capabilities in fundamental research in chemical and molecular sciences that support DOE’s mission to achieve transformational discoveries for energy technologies, while preserving human health and minimizing environmental impact. The Lab has integrated theoretical and experimental Core Capabilities and instrumentation to enable the understanding, prediction, and ultimately the control of matter and energy flow at the electronic and atomic levels, from the natural timescale of electron motion to the intrinsic timescale of chemical transformations.
Berkeley Lab has expertise in gas-phase, condensed-phase and interfacial chemical physics. State-of-the-art laser systems that generate ultrashort pulses of extreme-ultraviolet light; soft X-ray sources; photon and electron spectrometers; spectromicroscopy; in situ, operando and other capabilities are all used to advance the understanding of key chemical reactions and reactive intermediates that govern chemistry in realistic environments. The Lab has deep expertise in experimentation, simulation and theory aimed at a first-principles description of solvation and molecular reactivity in complex interfacial environments. The Lab is a world leader in momentum-imaging instrumentation, reaction microscopy, and theoretical methods that probe how photons and electrons transfer energy to molecular frameworks and provide critical knowledge in atomic, molecular and optical sciences needed to understand and ultimately control energy flow. Ultrafast attosecond and femtosecond probes enable studies of electron motion that may lead to reaction engineering at the atomic scale.

Berkeley Lab’s catalysis capabilities include basic research on homogeneous and heterogeneous chemical conversions for high efficiency and selectivity. The catalysis facility co-locates a suite of state-of-the-art instruments used for catalysis research and includes high-throughput dryboxes, a Micromeritics analyzer, flow UV-Vis spectroscopy, liquid chromatography, pressure reactors and FTIR instrumentation. The core strengths are in three pillars of catalysis: mechanisms, transformations, and environments that elucidate fundamental principles in catalysis and chemical transformations at the molecular level. Research on both the catalytic center and its environment advance the field from discovery to catalyst design.

The Heavy Elements Research Laboratory (HERL) has unique capabilities in electronic structure, bonding and reactivity of actinides, including the transuranic elements. The scientific personnel and instrumentation characterize, understand, and manipulate rare earth complexes for discovery and separation of alternative elements and critical materials, including those for energy storage, motors, solid-state lighting, and batteries.

Berkeley Lab has exceptional capabilities in solar photoelectrochemistry, photosynthetic systems and the physical biosciences. These photosynthetic and photoelectrochemistry capabilities, together with novel spectroscopies and in situ imaging methods that utilize photon energies from X-rays to infrared at high temporal resolution, enable elucidation of the structure and elementary mechanisms of biological and artificial photon-conversion systems. The deep understanding of artificial and natural photosynthesis forms a basis for efficiently engineered solar-conversion systems. Berkeley Lab is lead lab partner for the DOE Energy Innovation Hub devoted to the development of new photoelectrochemical approaches to fuel production, the Joint Center for Artificial Photosynthesis (JCAP).

Berkeley Lab leads the scientific community in the control and manipulation of the interaction of living and nonliving molecular systems by addressing the communication between live cells and organic/inorganic surfaces at the molecular level. The Chemical Dynamics and Molecular Environmental Science Beamlines at the ALS provide the pioneering application of vacuum ultraviolet and soft X-ray synchrotron radiation to critical problems in chemical dynamics and interfacial chemistry. The Ultrafast X-ray Science Laboratory (UXSL) develops laser-based ultrafast X-ray sources for chemical and atomic physics experiments and contributes to the knowledge base for future powerful FEL-based attosecond light sources.

This Core Capability is supported primarily by BES, with important contributions from ASCR. Other DOE contractors and SPP enable this Core Capability, which supports DOE’s mission to probe, understand and control the interactions of phonons, photons, electrons and ions with matter; and to direct and control energy flow in materials and chemical systems.
3. Chemical Engineering.
At Berkeley Lab, this Core Capability links basic research in chemistry, biology and materials science to deployable technologies that support energy security, environmental stewardship and nanomanufacturing. Leading capabilities are provided in the fields of chemical kinetics; catalysis; molecular dynamics; actinide chemistry; electronic, biomolecular, polymeric, composite and nanoscale materials; surface chemistry; ultrafast spectroscopy; crystal growth; mechanical properties of materials; metabolic and cellular engineering applied to recombinant DNA techniques that create new chemical processes within cells; and new methodologies for genomic and proteomic analysis in high-throughput production that enable gene libraries that encode enzymes for metabolic engineering.

Other program components provide the capability to translate fundamental research in catalysis, chemical kinetics, combustion science, hydrodynamics and nanomaterials into solutions to technological challenges in energy storage and efficiency, as well subsurface energy and environmental science. The Advanced Biofuels Process Demonstration Unit (ABPDU), supported by EERE and SPP, integrates biological and chemical unit operations through bioprocess engineering to understand and optimize processes for producing biofuels, renewable chemicals and proteins relevant to industry. Berkeley Lab also has expertise in chemical biology and radionuclide decorporation, necessary for characterizing mammalian response and developing sequestering agents for emergency chelation in humans in case of heavy-element or radioactive contamination.

Berkeley Lab is a leader in materials for advanced battery technology, focusing on the development of low-cost, rechargeable, advanced electrochemical devices for both automotive and stationary applications. This effort includes the collaborative JCESR program. The related field of fuel-cell research enables the commercialization of polymer-electrolyte and solid-oxide fuel cells for similar applications.

This Core Capability is supported by BES, ASCR, BER, EERE, and SPP, including the National Institutes of Health, DoD, universities, and industry. It supports DOE’s missions to foster the integration of research with the work of other organizations within DOE, as well as other agencies, and applies directly to DOE’s energy security and environmental protection mission, including solar and fossil energy, biofuels, and carbon capture and storage.

Berkeley Lab researchers develop experimental and theoretical techniques to discover, design, and understand new materials and phenomena across multiple time, length, and energy scales and in-situ and operando environments. These materials can have a direct and significant impact on solutions to grand challenges in energy, environment, and security.

In recent years, novel materials of interest at the Lab have included quantum materials, where quantum mechanics ultimately determine the nature of ordered phases and the transitions that take place between them. This includes weakly correlated topological phases such as topological insulators and Weyl and Dirac semi-metals, and materials that exhibit novel forms of magnetic, electronic and geometric/spatial order, specifically 2D materials such as graphene or van der Waals heterostructures. Berkeley Lab is interested in artificially engineered “metamaterials” that can be tailored in shape and size to be tuned at a sub-wavelength scale and have potential to bring solutions to real-time imaging that is limited by diffraction effects. Novel states of matter can be explored in the ultrafast time regime, particularly when the system is far from equilibrium. Another promising route to design novel materials is to take inspiration from biology with so-called bio-inspired hybrid nanostructured materials. Their unique properties can be derived from hierarchical architectures controlled over length-scales from nano– to macro dimensions.
Theory and computational simulations are critical to the discovery and design of new materials. Berkeley Lab researchers develop models for understanding, predicting and controlling complex materials with targeted properties. The new Center for Computational Study of Excited-State Phenomena in Energy Materials will develop new general software, theories, and methods to understand and predict excited-state phenomena in energy-related materials. Open access to analysis tools and computed information on known and predicted materials provided by the Materials Project helps the Lab to conduct theoretical work in high-throughput scenarios.

The characterization of properties and behavior including structure, function, and reactions, specifically at interfaces between various phases of matter enable Berkeley Lab researchers to understand how new materials may perform in various environments. Efforts rely on developing instrumentation for time-domain approaches in ultrafast spectroscopy, diffraction and quantitative microscopy. Advancing electron beam and scanning probe techniques operating in-situ and in-operando environments with near-atomic resolution is a key focus, and unique characterization tools include time-resolved angle-resolved photoemission spectroscopy for studies of materials far away from equilibrium as well as ultrafast electron diffraction.

The Joint Center for Energy Storage Research (JCESR) seeks to understand electrochemical materials and phenomena at the atomic and molecular scale, and to use this fundamental knowledge to discover and design next-generation energy-storage technologies. The ability to understand materials and chemical processes at a fundamental level should enable technologies beyond traditional lithium-ion batteries and store at least five times more energy than today’s batteries at one-fifth the cost. Berkeley Lab is a key partner of this hub, which is led by Argonne National Laboratory.

This Core Capability is primarily supported by BES, with important contributions by ASCR, EERE, and DoD, as well as other SPP sponsors from industry. It supports DOE’s missions to discover and design new materials and molecular assemblies with novel structures and functions through deterministic atomic and molecular scale design for scientific discovery, innovative energy technology and improved homeland security.

5. Earth Systems Science and Engineering.

Berkeley Lab’s Geosciences group, the largest team of its kind in the DOE complex, conducts fundamental research to understand, model, and influence the behavior of subsurface phenomena from nanometer to kilometer length. Developed with support from BES, the fundamental knowledge and capabilities are used to grow deployable technologies that enable the judicious use of important subsurface energy resources. The Lab has three fundamental BES-geoscience programs, in geophysics, geochemistry and isotope geochemistry, and also leads the Energy Frontier Research Center on Nanoscale Controls on Geologic CO₂ (NCGC). Fundamental theories about the interplay of belowground processes are coupled with new geophysical visualization methods to design monitoring tools and test predictive capabilities that improve use of subsurface resources. Cutting-edge analytical, characterization and simulation capabilities improve understanding of subsurface system behavior – over large spatial and temporal scales. Research in molecular and isotopic geochemistry queries fundamental aspects of mineral-fluid and fluid-fluid interactions, employing synchrotron X-ray and mass spectrometric analysis and molecular dynamics and \textit{ab initio} computational approaches. NCGC is directed at the molecular, nanoscale and pore scales to reveal properties and processes that affect the transport of supercritical CO₂ in subsurface environments and control trapping of CO₂ in the subsurface. The Lab creates world-unique experimental platforms to measure subsurface properties and processes, including the Center for Isotope Geochemistry, the Geosciences Measurement Facility, the Center for Computational Geophysics, and the Environmental Applied Geophysics Laboratory.
Complementing the fundamental research support provided by BES-geosciences, Berkeley Lab has a significant applied research portfolio to enable sustainable utilization and management of the subsurface, which supplies more than 80% of the nation’s primary energy, including from fossil fuels and geothermal systems. The subsurface also provides a vast resource for disposal of energy waste products (e.g., CO₂, nuclear waste, produced water). Understanding how fundamental processes influence reservoir-scale processes – and how to adaptively manipulate them for beneficial utilization while minimizing environmental risks – is a significant challenge, given the complexity, remoteness, and elevated temperature/pressure of subsurface reservoirs. Berkeley Lab’s applied research, supported by EERE-Geothermal, FE Clean Coal, FE Oil & Gas, NE Spent Fuel and Waste Disposition, and by several significant SPPs, seeks to realize a significant increase in geothermal resources, transition effectively to a clean energy future by pairing fossil energy use with carbon sequestration, ensure that groundwater is protected from contamination, and advance safe and cost-effective solutions to large-scale utilization of the subsurface.

Specific research elements of Berkeley Lab’s applied subsurface energy program include the control of subsurface fluid flow and reactions, the characterization and manipulation of subsurface stress and induced seismicity, the development and application of novel sensing and monitoring tools, and the use of risk assessment frameworks for safe implementation and mitigation. This subsurface program is well aligned with the DOE Subsurface Crosscut Initiative (SubTER), which the Lab co-leads for the nation. The Lab is also active in various subsurface energy field observatories, such as FE’s CCS demonstration tests, the Brine Extraction Storage Test (BEST), and the Frontier Observatory for Research in Geothermal Energy (FORGE).

In 2016, Berkeley Lab’s geoscientists helped to solve several relevant challenges to subsurface energy utilization. For example, Lab scientists provided significant scientific and technical support to the State of California to resolve the gas well blowout disaster at Aliso Canyon, and they contributed cleanup efforts in the contaminated Fukushima region via data analysis and cesium transport modeling. Berkeley Lab is also studying the seismic risk of nuclear power plants, a project that involves development of new transformational modeling tools for earthquake rupture simulation and impacts on buildings. A recently awarded exascale application project led by the Lab will take these modeling tools and develop a computational framework specifically for use on future exascale systems. These capabilities align with plans for a substantial research program on the advanced design, assessment, and maintenance of the Nation’s critical infrastructure. Another new exascale project awarded to the Lab seeks to develop an exascale predictive capability for the coupled hydrological, chemical, thermal, and mechanical processes that control the success or failure of many energy related endeavors including geologic CO₂ sequestration, geothermal energy and nuclear waste isolation.

Biological and Environmental Sciences

Many of the most pressing 21st Century energy and environmental challenges require an ability to understand, predict, and influence how change unfolds to make both the natural world and human society more resilient. To do so requires a new and deeper understanding of Earth’s complex processes. Berkeley Lab is transforming our ability to decipher and map the vast networks of these interconnected systems, the scale of which range from nanometers to thousands of kilometers, and from nanoseconds to centuries. This enables our ability to predict how environmental changes impact biological systems; harness biology for sustainable energy and other valuable products; predict how terrestrial systems feedback to climate; and improve predictions of watersheds, ecosystems and climate interactions for a greater understanding of global change for DOE energy and environment missions.

6. Biological and Bioprocess Engineering.

Berkeley Lab’s strengths in biological systems science are complemented by unique capabilities for biological and bioprocess engineering to translate fundamental science discoveries to use-inspired...
solutions for energy and environment. The Lab has world-renowned capabilities in synthetic biology, technology development for biology, and engineering for biological process development. By leveraging resources such as the JGI, the Joint BioEnergy Institute (JBEI), DOE Systems Biology Knowledgebase (Kbase), ENIGMA, the ALS, the Molecular Foundry and NERSC, Berkeley Lab can develop the new technologies and processes needed to create renewable fuels and chemicals, remove environmental contaminants and support biosequestration of carbon.

The ABPDU provides capabilities for scale-up of biofuels pretreatment, saccharification and fermentation methods. In collaborations with national labs and with industry, this facility develops new and optimizes existing processes for biofuels and bio-based chemicals and materials processes. In FY16, the ABPDU initiated 10 new projects with small companies, three of which were awarded through EERE’s Small Business Voucher Program, and in the past three years, the ABPDU has partnered with 29 companies through CRADA or SPP agreements.

JBEI’s biofuels successes have given rise to the Agile BioFoundry (ABF) at Berkeley Lab, with the potential to transform manufacturing practices through advanced bioconversion technologies in support of a bio-based economy. Funded initially with LDRD and proof-of-concept DARPA funding, the ABF was piloted by DOE’s Bioenergy Technologies Office (BETO) in FY16 with considerable industry input to demonstrate rapid improvement over the state of the art for production of adipic acid. NREL, PNNL, and Sandia also participated in the pilot project. Led by Berkeley Lab, the ABF consortium was established in 2017 to leverage capabilities across the national laboratory system; it includes: Ames, ANL, INL, LANL, NREL, ORNL, PNNL, and SNL. The ABF integrates computer-assisted biological design, advanced metabolomics and proteomics techniques, machine learning, techno-economic and sustainability analysis, and process integration to optimize biological process design and develop methods for predictable scaling. The ABF consortium will continue to engage with private sector stakeholders through its industry engagement task and establishment of an advisory board comprised of experts from companies in the bio-based products and biological computing fields. This engagement task is intended to identify the highest priority R&D barriers in biomanufacturing that should be addressed by the ABF, as well as to develop metrics for success of ABF’s research and development relevant to industry.

EERE is the primary supporter of this Core Capability, building upon capabilities and programs established with BER funding. Other key sponsors include industry and other SPP; anticipated sponsors include USDA, DoD, and the NIH. This Core Capability supports DOE’s objectives to increase commercial impact through: the transition of national laboratory-developed technologies to the private sector; utilization of national laboratory facilities and expertise; and demonstration and deployment for the economic, energy, and national security of the nation.


As described below, Berkeley Lab sustains leading capabilities in systems biology, genomics, biodesign, structural biology and imaging at all length scales (from protein structure to ecosystems). The Lab is also a national leader in microbial biology, cell biology, plant biology, microbial community biology, environmental sciences, and computational biology. The capability is further enhanced by instrumentation at the ALS, DOE JGI, the Molecular Foundry, NERSC and JBEI. Berkeley Lab has the capability to characterize complex microbial community structure and function; manage highly complex biological data; visualize biological structure; and produce large-scale gene annotation.

The DOE Systems Biology Knowledgebase (http://kbase.us/) is an open source, open access software and data platform designed to meet the grand challenge of systems biology—predicting and designing biological function from the biomolecular (small scale) to the ecological (large scale). The project’s long-term goal is to understand how plants and microbes interact with and affect each other and
environmental processes, and how these interactions could be harnessed for sustainable bioenergy and environmental solutions. KBase enables researchers to collaboratively generate, test, compare, and share hypotheses about biological functions; perform large-scale analyses on scalable computing infrastructure; and combine experimental evidence and conclusions that lead to accurate models of plant and microbial physiology and community dynamics. The KBase collaboration (which includes groups at LBNL, ANL, ORNL, BNL, and several universities) is committed to supporting the optimal use and dissemination of data and tools generated by DOE programs, particularly by the main Science Focus Areas, Bioenergy Research Centers, and user facilities.

JGI and KBase are developing complementary but integrated high-performance tools that provide Users with the ability and infrastructure to explore complex and diverse datasets to extract deeper biological insights. Through joint strategic leadership, joint tactical teams and frequent communication, both institutions are partnering to accomplish the goals laid out on a joint roadmap whilst leveraging capabilities across Berkeley Lab. Successful partnership between JGI and KBase will enable users to seamlessly access and analyze data on scales ranging from single genes and individual genomes to metagenomes to systems level modeling and understanding.

The Joint BioEnergy Institute (JBEI) is one of the three DOE BRCs whose mission is to advance science, engineering and technology to support conversion of lignocellulosic biomass to liquid transportation fuels and bioproducts. Using molecular, computational and robotic technologies, JBEI has successfully altered biomass composition in model plants and crops and demonstrated that ionic liquids can deliver near-complete dissolution of plant biomass to facilitate its conversion to sugars needed to produce energy-rich fuels. The production of commodity chemicals from biomass brings environmental and economic benefits as well as the possibility of producing diverse, novel molecules through biological conversion pathways that are challenging or currently impossible using chemical synthesis approaches. Industry realizes the economic potential of such breakthroughs, and the licensed technologies from JBEI’s activities are steadily coming out of the strong industrial affiliate program.

The multi-institutional Berkeley Lab-led BER-funded SFA called ENIGMA (Ecosystems and Networks Integrated with Genes and Molecular Assemblies) advances an understanding of microbial biology and the impact of microbes on their ecosystems. By linking environmental microbial field studies to powerful meta-functional genomic and genetics tools, the identity and diversity of microbes along gradients of geochemical parameters can be understood, enabling predictions of how environmental perturbations may affect microbial community structure and their ecosystems. ENIGMA’s computation efforts are aimed at integrating diverse, complex, large datasets for studies of dynamic modular microbial architectures across scales, from regulons (groups of genes regulated by one protein) to full community assemblages.

BER is the primary sponsor; others include EERE, NIH, DoD, industry, and other SPP sponsors. This Core Capability supports DOE’s mission to: (1) obtain new molecular-level insight for cost-effective biofuels; (2) make discoveries for DOE’s needs in climate, bioenergy, and subsurface science; (3) coordinate bioenergy, climate and environmental research across DOE’s applied technology offices.


Physical, chemical, biological and atmospheric interactions regulate the geochemical flux of life-critical elements, influence contamination migration, control agricultural production, and influence the quality and quantity of water. These interactions also influence water and energy security (including hydropower and biofuel crop growth) as well as greenhouse gas feedbacks to climate systems, including carbon and methane. With support from BER, Berkeley Lab is developing a predictive understanding of watershed function, including the interplay of multi-scale biotic-abiotic interactions spanning from
bedrock to canopy (including between the saturated and unsaturated subsurface, soils and vegetation compartments, terrestrial-aquatic subsystems) and along significant environmental gradients.

Berkeley Lab’s Watershed Function SFA is developing a predictive understanding of how mountainous watersheds retain and release downgradient water, nutrients, carbon, and metals. This significant BER Subsurface Biogeochemistry SFA is exploring how early snowmelt, drought, and other disturbances will influence mountainous watershed dynamics at seasonal to decadal timescales. The Watershed Function project is being carried out in a headwater mountainous catchment of the Upper Colorado River Basin, which provides water for 1 in every 10 Americans, hydropower to millions, is host to a range of redox sensitive contaminants, and irrigates 4.5 million acres of agricultural land. Berkeley Lab has developed a ‘community watershed’ here, attracting collaborators from 13 universities, 2 companies and 2 non-profit institutions, who bring unique and complementary strengths to key BER challenges investigated at the site. To improve prediction of future watershed function, scale-adaptive modeling approaches are being developed to simulate hydrological and biogeochemical dynamics in response to climate/weather perturbations. This first-of-a-kind watershed model will be able to simulate fine scale processes (including microbial) when and where needed, as well as inform operational models in the Colorado River Basin. The new capability is expected to be particularly useful for understanding how watersheds will respond to increasingly frequent extreme events and for exploring the interplay between climate, water supplies, biogeochemistry and energy resources. New nimble and networked observation platforms are being deployed across the watershed, which are elucidating hydrogeological, ecohydrological, and organic-mineral interactions that influence how the watershed is responding to perturbations. BER supports the Watershed Function SFA and several of the collaborating university projects.

Within the national lab network, Berkeley Lab is a key partner in multi-institutional Interoperable Design of Extreme-Scale Application Software (IDEAS) project funded by DOE Office of Science (BER and ASCR) as well as the Advanced Scientific Computing for Environmental Management (ASCEM) project funded by DOE EM. Berkeley Lab also collaborates with the Japanese nuclear consortium JAEA and UC Berkeley on the topic of Fukushima contamination. This capability is sponsored by BER, EM, LM, DoD/DHS/ EPA, CA State Agencies, UC, SBIR and ARPA-E; it contributes to DOE’s linked energy and environmental security mission. Closer to home, Berkeley Lab has also used BER-developed insights and approaches during this reporting period to explore the potential for microbiologically mediated release of metal contamination in riverbed sediments associated with the Aug 2015 Animas River (King Mine) spill in Colorado.

9. Climate Change Science and Atmospheric Science.

Berkeley Lab has developed an internationally recognized program in theoretical, empirical, and computational climate and atmospheric science. The Lab continues to make major advances in the theory governing how atmospheric convection, one of the fundamental processes governing the equilibrium of Earth’s climate, will respond to further warming of the environment. The Lab has complemented this work with novel observations of how the terrestrial ecosystem serves as a critical carbon sink and how elevated concentrations of greenhouse gases are leading to measurable increases in the atmospheric greenhouse effect. Lab scientists integrate this information to help DOE produce the most advanced models of the Earth system and to utilize those models to project the possible physical and biogeochemical impacts of further global climate change.

Berkeley Lab conducts internationally recognized research on advancing the understanding and prediction of ecosystem responses and feedbacks to climate. The Lab leads the Next Generation Ecosystem Experiment in the Tropics (NGEE-Tropics), focused on a predictive understanding of how tropical forest carbon balance and climate system feedbacks will respond to changing environmental drivers. NGE-Tropics is taking advantage of the El Niño-Southern Oscillation to measure and model
drought impacts on tropical forests, and established Pan-Tropical sites and partnerships. The Lab is advancing a representative, process-rich tropical forest ecosystem model (Functionally Assembled Terrestrial Ecosystem Simulator – FATES), extending from bedrock to the top of the vegetative canopy-atmosphere interface, in which the evolution and feedbacks of tropical ecosystems in a changing climate can be modeled at the scale/resolution of an ACME grid cell. NGEE Tropics has also launched extensive ModEx field observations in Panama, Puerto Rico, and Manaus and is leading international workshops on partnerships to form a pantropical observational network following NGEE-Tropics protocols. NGEE Tropics is actively sharing data and models with other DOE projects including Ameriflux, NGEE Arctic, and ACME, as well as LBA and ForestGEO.

Berkeley Lab is a key partner in the NGEE-Arctic project, contributing its expertise in environmental geophysics, soil biogeochemistry and microbial ecology, and mechanistic modeling of ecosystem-climate feedbacks. In 2016, the team developed and used novel above-and-below ground coincident monitoring systems to investigate permafrost through canopy dynamics; developed several new Seward Peninsula field study sites; and advanced several capabilities to improve prediction of ecosystem feedbacks to climate. The team also explored how soils will respond to warming in situ, using controlled manipulation experiments in the field. One experiment was performed in Barrow, Alaska, as part of the NGEE-Arctic project, and one in California as part of the TES SFA. These warming experiments are closely coupled to modeling activities, which will result in more robust understanding and tools for prediction.

Berkeley Lab also leads the Ameriflux program, a network of over 120 sites in North and South America that measure ecosystem atmosphere fluxes of carbon, water and energy. During the past year, the Berkeley Lab Ameriflux site data were downloaded by thousands of scientists from around the world. Key strategic thrusts associated with the terrestrial ecosystem science include dynamic vegetation observation and modeling, and together with subsurface science, we are developing terrestrial community observatories that enable scientific and modeling advances. Ameriflux has been renewed through 2020 with a significant post-award augmentation for Data Management. Berkeley Lab and Ameriflux co-led production, with international partners, of FLUXNET2015—the first global synthesis data product for ecosystem fluxes since 2008. Eighty Ameriflux sites were included. Since December 2015, it has been used by more than 250 scientists from six continents. The Lab organized several events to commemorate the 20th Anniversary of the Ameriflux Network, including a PI Meeting and Data/Tech workshop, AGU Town Halls and science sessions, and a special issue of the journal Agricultural and Forest Meteorology.

Berkeley Lab is one of the primary science centers studying the atmospheric carbon cycle and land-atmosphere interactions, and currently leads several major BER projects in the Atmospheric System Research (ASR) and Atmospheric Radiation Measurement (ARM) programs. The Lab developed and operates the carbon measurement capabilities for ARM. With PNNL and LLNL, Berkeley Lab co-leads development of the emerging land-atmosphere-cloud interactions theme, which couples land surface and atmospheric dynamics to address cloud and precipitation biases in DOE climate models.

Berkeley Lab actively engages in DOE’s flagship ACME project, with its integrated assessment models to create a fully coupled Earth system model that can project the future interactions among energy, food, water resources and climate using state-of-the-science treatments of physical, chemical and biogeochemical processes. Lab researchers are members of the ACME council, land model group co-lead, and leads and task leads for NERSC exascale applications. The Lab launched the Calibrated and Systematic Characterization, Attribution and Detection of Extremes (CASCADE) project to detect and attribute the influence of anthropogenic climate change on past, current and future climate trends through the application of DOE’s uncertainty quantification capabilities integrated with new highly parallel computational “pipelines.” CASCADE’s primary objective is to improve our ability to predict extreme events and understand the causes in long-term changes in the severity and frequency of these events. The Lab also leads a DOE SciDAC project constructing models telescopend through advanced
numerical techniques to simulate climate phenomena with high resolution and physical fidelity. Primary support for this Core Capability comes from BER and ASCR. Additional research in Earth observations from space is obtained through the NASA and the state of California.

Computing and Mathematics

10. Advanced Computer Science, Visualization and Data.

Berkeley Lab is a leader in computer architecture research, with expertise in low-power parallel processor design, optical interconnects and memory systems unique within DOE. The partnership with Sandia in deploying DOE’s Computer Architecture Lab (CAL) enables Berkeley Lab to play a critical role in the Design Space Exploration activity for the Exascale program, which aims to develop energy efficient and effective processor and memory architecture R&D.

Berkeley Lab is also a leader in performance analysis and algorithms research, with multiple award-winning papers on application performance analysis and the efficient use of emerging computer architectures for scientific applications. The Lab and UC Berkeley established and continue to lead the field of automatic performance tuning research, as shown by recent work on improving the performance of the nuclear structure code BigStick by a factor of 7X on the Intel Knight’s Landing (KNL) nodes of the NERSC Cori system. Recent progress in designing parallel graph-based algorithms for sparse matrix sparse vector multiplication, a key piece of many machine learning algorithms, has produced speedups of more than 49X on KNL nodes. This expertise finds its way into widely deployed tools, for example, the Roofline Model, a visually intuitive performance model used to bound the performance of various numerical methods and operations running on multicore, manycore, or accelerator processor architectures, first developed in 2009, has been incorporated into an Intel performance tuning tool. Use of this tool has led to some significant speedups in application performance on the NERSC Cori system.

The design and deployment of a highly usable, energy-efficient exascale system presents research challenges in programming languages, system software and tools. Berkeley Lab is a global leader in programming languages and compilers for parallel machines, and utilizes this experience in the design of programming models for future systems. For example, in 2016, Katherine Yelick was elected to the National Academy of Engineering for software innovation and leadership in high-performance computing. Both the Lab’s Unified Parallel C++ and Global-Address Space Networking (GASNet) runtime system are broadly deployed by computing-system vendors, government agencies and academic institutions. This programing model is especially powerful for problems that require random access to large data sets or memory, such as the HipMer extreme scale genome assembler. This effort will also play an important role in the Exascale Project Software Technologies activity.

While ASCR’s main focus – and ours – is on exascale technology, we have also begun to explore quantum computing, neuromorphic computing and alternative devices to address the anticipated end of transistor density scaling. For quantum computing, our work has focused on generalizing algorithms for small numbers of non-error corrected qubits with application to chemistry and materials.

Berkeley Lab is also a leader in the development of new capabilities in high performance and data-intensive visualization and analysis. Key new developments include: the SENSEI \textit{in-situ} visualization and analysis infrastructure, where the visualization algorithms run concurrently with simulations; and more scalable algorithms to deal with increasingly larger datasets, such as improvements to Delaunay and Voronoi tessellation algorithms for cosmological simulation data. By using Convolutional Neural Networks, on conventional and novel neuromorphic hardware, lab researchers have developed sophisticated feature detection pipelines and tools for scientific image retrieval based on pictorial similarity.
Berkeley Lab is a pioneer in scalable solutions for scientific data, including management, curation, quality-assurance, distribution and analysis. Some recent work has complemented the computationally efficient Adaptive Mesh Refinement (AMR) methods developed by our Applied Mathematics researchers by extending previously developed indexing and querying techniques to the more complex datasets generated by AMR. Factors of up to 500X speedup were achieved over non-AMR aware algorithms; similarly, by extending I/O methods to incorporate new buffering techniques and use of new data storage technologies, such as the NERSC Burst Buffer, almost an order of magnitude speedup could be achieved. A state-of-the-art framework called the Berkeley Data Cloud is being developed; it enables users from different research communities easy and fast access to nuclear radiation data and analyses collected by the advanced multi-sensor radiation detection systems for airborne (ARES and DTRA UAV research) and mobile terrestrial (RadMAP) platforms that are being deployed by the applied nuclear physics programs. For the Ameriflux program, where ecosystem-level field sites acquire continuous measurements from a large number of sensors at high temporal resolution, the Lab heads up the data assimilation, curation and distribution services. Data collected at individual sites is sent to an archive, where processing creates high quality, standardized datasets to be distributed to a variety of data users. Berkeley Lab is a partner in the FE funded Institute for the Design of Advanced Energy Systems (IDAES) project that is developing a next generation modeling and optimization platform to aid in the design of novel energy systems. In IDAES our role is helping lead the Software Architecture, Algorithms, and Distributed Computing tasks including: system architecture, data management and workflow, and parallel computing.

Berkeley Lab is a leader in troubleshooting and performance-analysis tools for complex, distributed applications, such as the PERFormance Service Oriented Network monitoring ARchitecture (perfSONAR) application, which is now deployed at over 2,000 sites worldwide in national laboratories, commercial and research networks, universities, and corporations. ESnet and Berkeley Lab computer scientists work with researchers around the globe to meet the distributed computing and networking needs of the next generation of DOE science experiments. ESnet’s On-Demand Secure Circuits and Advance Reservation System (OSCARS) technology, deployed in over 50 networks worldwide, operates like a dynamic expressway, creating uncongested paths between endpoints.

ASCR is the primary support for this Core Capability, and significant benefits accrue for all SC offices and other elements of DOE, as well as strategic partners such as the DoD. This capability supports SC’s mission to deliver computational and networking capabilities that enable researchers to extend the frontiers of science and to develop networking and collaboration tools and facilities that enable scientists worldwide to work together and share extreme-scale scientific resources.


Berkeley Lab has world-leading capabilities for developing mathematical models, algorithms, tools and software for high-performance computing. The Lab has a large pool of highly recognized experts in applied mathematics, many of whom are SIAM Fellows and/or members of NAS and NAE.

Berkeley Lab has unsurpassed expertise in algorithms for modeling and simulating compressible, incompressible, and low-Mach-number flows in many applications, from terrestrial combustion processes, to ice-sheet formation and retreat, to nuclear flames in supernovae. AMR techniques pioneered at the Lab are globally recognized as a key enabling technology, and the AMR Co-Design Center for the Exascale Computing Project is based at the laboratory. Coupled with AMR algorithms, the Lab’s hierarchical structured-grid finite difference capabilities can solve turbulent flow problems 10,000 times faster than previous techniques. Researchers have recently applied AMR techniques to develop a shallow water model that can be incorporated into a full climate model, in an approach that makes simulations possible at a resolution that would be infeasible with a uniform mesh.
Berkeley Lab and UC Berkeley have developed high accuracy algorithms based on Voronoi implicit interface methods, interfacial gauge methods, and high-order Discontinuous Galerkin (DG) methods. These algorithms can follow the evolution of multiple moving interfaces and boundaries for problems in grain evolution in materials, multiscale mixing and transport, industrial liquid foams over five orders of magnitude in space and time, and design optimization for vertical axis wind turbines.

The Center for Applied Mathematics for Energy Research Applications (CAMERA), an integrated, cross-disciplinary center aimed at developing and delivering the fundamental new mathematics required to support DOE user facilities, has delivered numerous advances. The 2016 BESAC Facility Upgrade Assessment cited CAMERA as “highly effective” in enabling researchers to analyze light source data. For example, a new multi-tiered iterative phasing algorithm to reconstruct structural information from single-particle diffraction data by simultaneously determining the states, orientations, intensities, phases, and underlying structure in a single iterative procedure. In conjunction with staff from our Advanced Computer Science, Visualization and Data core capability and others, CAMERA has also delivered an integrated software/algorithmic framework called Xi-CAM, designed to capitalize on high throughput experiments, and provide real-time pipeline processing of ptychography and other experimental data, enabling high throughput, compression, analysis, and resolution as well as rapid feedback to end users.

In numerical linear algebra, Berkeley Lab is the only SC lab whose researchers have expertise in large-scale eigenvalue calculations and direct solutions in sparse matrix computation. For example, in 2016, Sherry Li was named a SIAM Fellow for advances in the development of fast and scalable sparse matrix algorithms and fostering their use in large-scale scientific and engineering applications. Leveraging existing methods, new eigensolvers have been developed and incorporated into the Quantum Espresso suite of density functional applications that show a factor of two speedup over existing state-of-the art methods. To prepare for future computer architectures with many more components and much higher degrees of parallelism, previous work on efficient algorithms for sparse structured matrices has been generalized for resiliency.

Berkeley Lab’s mathematics work is a point of leverage for exascale science impact. The algorithms and models are designed for parallel scalability and to reduce expensive data movement, with special attention to the hardware features emerging in next generation systems. They are incorporated into open source software libraries and frameworks that are used at NERSC and other centers across DOE, and will enable higher resolution, more details, and new models of scientific phenomena.

These capabilities and their applications are sponsored primarily by ASCR, with support from other DOE program offices and SPP. These capabilities support DOE missions in fusion energy science, biological and environmental research, high-energy physics, nuclear physics, basic energy sciences, environmental management and fossil energy. These capabilities also support the development of mathematical descriptions, models and algorithms to understand the behavior of climate, living cells, and complex systems related to the DOE mission areas of energy and environment.

### 12. Computational Science.

Berkeley Lab is a leader in connecting applied mathematics and computer science with research in many scientific disciplines, including biological systems science, chemistry, climate science, materials science, particle and nuclear physics, subsurface science, fossil energy, environmental management and all Core Capability areas described in this Plan. The Lab has a successful track record of effectively integrating these research areas in conjunction with high-performance computing resources to obtain significant results in many areas of science and engineering. Within the national lab network, Berkeley Lab plays a very visible role in the SciDAC Program. Out of the 19 science partnership projects, Berkeley Lab is involved in 11 of them, providing advanced computer science methods and robust applied math
techniques and algorithms for enabling and accelerating scientific discoveries. These successes also
make use of the results from three SciDAC Institutes related to our Applied Math and Advanced
Computer Science, Visualization and Data core capabilities. Furthermore, Berkeley Lab plays key roles in
providing computer science and applied math expertise in twelve Application Development activities in
the Exascale Computing Project. A few of the many examples of this work are illustrated in the
remainder of this section.

As mentioned in the Climate Change Science core capability, an extensive collaboration with domain
scientists, applied mathematicians and computer scientists is now focused on large-scale climate science
efforts. The relationship includes interactions with SciDAC institutes SUPER, FastMATH and SDAV to
ensure applications are scalable and achieve high performance on next generation computing platforms,
which will enable novel climate science research at unprecedented scales and fidelity.

To increase the speed and reduce the errors in identifying astronomical objects, computational
scientists at Berkeley Lab have teamed with the intermediate Palomar Transient Factory to construct a
real-time analysis pipeline consisting of machine-learning methods to perform basic calibration and
image differencing. Recently, an exceptionally rare gravitationally-lensed Type 1a supernova was
detected using this pipeline, and a method for identifying more of these events from existing and future
surveys proposed. Gravitationally-lensed Type 1a supernova may be key to measuring the rate of the
Universe’s expansion with unprecedented accuracy and distribution of matter in the cosmos. On a
related note, Julian Borrill was awarded the NASA Exceptional Public Achievement Medal for conceiving
and implementing the mission-critical high performance computing system for Planck data analysis.

The Integrated Microbial Genomes (IMG) system contributes improving the overall quality of microbial
genome and metagenome data. It integrates genomes from all three domains of life, as well as plasmids,
viruses and genome fragments, and provides tools for analyzing and reviewing the structural and
functional annotations of genomes in a comparative context. With about 50,000 datasets, the IMG is
one of the largest publicly available data management and analysis systems for microbial genome and
metagenome datasets. The system has more than 15,000 registered users from 89 countries across 6
continents, has contributed to thousands of published papers and has served as a tool for teaching
genome and metagenome comparative analysis at numerous universities and colleges around the globe.

In terms of presenting computational science tools to new audiences, Berkeley Lab supports the Carbon
Capture Simulation Initiative (CCSI), which has deployed state-of-the-art computational modeling and
simulation tools to accelerate the commercialization of carbon-capture technologies from discovery to
development, demonstration and ultimately the widespread deployment to hundreds of power plants.
By developing the interface and workflow tools of this comprehensive, integrated suite of validated
science-based computational models, this effort has provided increased confidence in designs, reducing
the risk associated with incorporating multiple innovative technologies into new carbon-capture
solutions. The CCSI Toolkit received an R&D 100 award in 2016.

Key collaborations connected with DOE’s Energy Frontier Research Centers and Hubs continue, targeting
gas separation and storage, carbon capture and sequestration, solar energy and batteries. The
mathematical methods and computational tools developed also have applications in many other
scientific domains, such as improving catalysts for hydrogen fuel cells and storage.

Although ASCR is a key source of support for this Core Capability, all SC offices sponsor computational
applications and software development for their respective areas of science. Other federal agencies
such as NASA and DoD also benefit from and contribute to the research effort. This Core Capability
supports all of DOE’s science, energy, environmental and security missions. For SC’s discovery and
innovation mission, it provides the mathematical models, methods and algorithms to enable scientists
to accurately describe and understand the behavior of complex systems.
13. Cyber and Information Sciences.

Berkeley Lab conducts research into a broad array of cyber and information sciences, most recently, including security in high-performance computing environments, security of high-throughput networks, security of “open science” computing workflows, cybersecurity for the power grid, and data provenance.

In addition, ESnet provides an integrated set of cyber security protections designed to efficiently protect research and operational data while enabling cutting edge research. ESnet’s unique 100G SDN network testbed provides an international research platform for cybersecurity research at all network layers. The Lab leads the world in developing technologies to optimize science data transfers across local and wide-area networks, the “Science DMZ,” and has championed this concept across the national and international research and education community. Investigation of applying the “Science DMZ” concept to data sets with privacy and security sensitive data is an ongoing effort. The Lab also conducts fundamental research in software-defined networking and network function virtualization forensics tools.

The “Bro” network security analysis framework, started at Berkeley Lab in the mid-1990s to monitor network traffic in open scientific environments, is now deployed in National Labs, major universities, supercomputer centers and, particularly through the Corelight (née Broala) commercial spinoff, Fortune 100 companies. Bro has recently been adapted for 100 Gbs speeds to enable scaling for the next generation of networks.

ASCR and OE (CEDS) are the primary support for this Core Capability, with additional support from EDER, OCIO, NNSA, and NSA. Significant benefits accrue for all SC offices and other elements of DOE, as well as strategic partners such as the DoD. This capability supports SC’s mission with disciplines, technologies and practices designed to protect, analyze and disseminate information from electronic sources, including computer systems, computer networks and sensor networks.

High Energy and Nuclear Physics


Berkeley Lab has a long record of excellence in particle physics and cosmology, with two premier programs: in the Energy Frontier on the ATLAS experiment, with many contributions and leadership roles over more than two decades; and in the Cosmic Frontier, where the Lab is leading next-generation projects in both dark energy and dark matter, and developing technologies for a future ground-based CMB polarization experiment to study inflation. LBNL has smaller, focused efforts on the Intensity Frontier, with leading contributions to the very successful Daya Bay neutrino experiment, a growing effort on the DUNE experiment, and key contributions to the Mu2E experiment.

LBNL’s experimental program is fully aligned with the P5 roadmap, and is enabled and enhanced by our traditional strengths in instrumentation and detector R&D, a strong theory group and increasing strengths in software and computation.

On the Energy Frontier, Berkeley Lab has played leading roles in the ATLAS pixel and silicon strip tracking detectors, computing and software systems, and physics analysis. The Lab pioneered the pixel development and led the international ATLAS pixel project. Physicists and computational scientists led the development of the ATLAS software framework. Lab scientists have lead roles in all aspects of ATLAS, including Physics Coordinator (Einsweiler, 2012-13), Deputy Spokesperson (Heinemann, 2013-17), Upgrade Coordinator (Einsweiler, 2015-19) and Simulation Convenor (Marshall, 2014-16). Lab scientists will have lead roles in both the pixel and strip inner tracking detectors for the HL-LHC ATLAS upgrades, with Lab staff serving in management positions in US-ATLAS and the international ATLAS upgrade teams.
The Lab now leads the design and construction of the Dark Energy Spectroscopic Instrument (DESI), a Stage IV BAO experiment to create the largest 3-D map of the universe, with over 20 million galaxies, successfully passing CD-3 in Spring 2016.

A critical element of Berkeley Lab’s leadership has been the development of advanced detectors. Red-sensitivity charge-coupled devices (CCDs) were invented in our MicroSystems Lab (MSL) and are the technology of choice for all Stage III and IV dark energy experiments, including BOSS, the Dark Energy Survey (DES), DESI and the Large Synoptic Survey Telescope. The Lab also developed detectors and a multiplexed readout for cosmic microwave background (CMB) measurements, including the South Pole Telescope (SPT) and POLARBEAR. The POLARBEAR project, led by Berkeley Lab Faculty Scientist and PI Adrian Lee, was commissioned in Spring 2010 and produced the first direct detection of CMB polarization in late 2013. POLARBEAR is now expanding into the Simons Array, with three identical telescopes with advanced multichroic polarization detectors, also invented at Berkeley Lab. A recent gift of $40M from the Simons Foundation will further extend this to become the Simons Observatory, encompassing both the Simons Array and the ACT experiment. Two LDRDs have been awarded to support the development of CMB detectors, readout and polarization modulators at LBNL, paving the way forward for the future CMB-S4 experiment.

LBNL was the lead lab for the Large Underground Xenon (LUX) experiment, and managed the science operations at the Sanford Underground Research Facility in South Dakota. LUX completed data taking in 2016, releasing new results that provide the most sensitive limits in the search for dark matter to date. LUX was successfully decommissioned and removed from SURF, making way for LZ, which was selected for the Generation 2 Dark Matter initiative at DOE HEP in 2014 with Berkeley as the lead lab. LZ was awarded CD3 in February 2017, and will be installed at SURF in 2020.

On the Intensity Frontier, Berkeley Lab provides scientific and computing leadership, as well as project management, for the Daya Bay reactor-based neutrino oscillation experiment. Both the Daya Bay U.S. spokesperson and U.S. operations manager are from Berkeley Lab. Daya Bay made the first observation of the third neutrino mixing angle and has the most precise measurements to date. The Daya Bay project received a DOE award for excellence in project management in 2013; the co-spokespersons, Kam-Biu Luk and Yifang Wang, have been awarded the 2014 APS W.K.H. Panofsky Prize and the 2016 Breakthrough Prize in Fundamental Physics. Berkeley Lab’s neutrino group is transitioning to the DUNE experiment, with key contributions to protoDUNE and a leadership role in the near detector. LBNL is also making key contributions in reconstruction, simulation and detector prototyping for the Mu2e experiment at Fermilab.

An increasingly important aspect of the LBNL program is computation; we have taken a leading role in software, simulation and computing for ATLAS, Daya Bay, Mu2e, BOSS, DESI and CMB experiments, and have successfully leveraged LBNL resources at NERSC and the LBNL Computing Research Division for HEP. The Center for Computational Excellence has provided additional resources to help take advantage of the NERSC HPC for HEP, and we have been successful in competing for other resources from ASCR.

The Berkeley Lab Theoretical Physics Group is closely integrated with the UC Berkeley Center for Theoretical Physics, and plays a crucial role in our particle physics program, working with experimentalists to define future programs and develop strategies for data analysis. The Particle Data Group provides a unique service to the international physics community through its compilation and analysis of data on particle properties.

DOE’s HEP is the primary sponsor of this Core Capability, with important contributions from ASCR, NNSA, NASA, NSF, and DHS. It supports DOE’s missions to understand the properties of elementary particles and fundamental forces at the highest energy accelerators; the symmetries that govern the interactions of matter; and obtain new insight on matter and energy from observations of the Universe.
15. Nuclear Physics.

Since the Lab’s inception, nuclear science has been a Core Capability. Current programs provide world leadership in neutrino research, heavy-ion physics, nuclear structure, and nuclear instrumentation.

In the study of neutrinos, Berkeley Lab’s critical role in the discovery of neutrino oscillations at the Sudbury Neutrino Laboratory has been widely recognized. KamLAND and IceCube resulted in the first observations of geo-neutrinos and ultra-high-energy cosmic neutrinos, respectively. Experiments also search for the rare nuclear process known as neutrino-less double-beta decay, which will demonstrate if the neutrino is its own antiparticle, provide information on the absolute neutrino mass scale, and determine if lepton number is conserved. Berkeley Lab scientists are playing important roles in the Majorana Demonstrator (MJD) SNO+, and the Cryogenic Underground Observatory for Rare Events (CUORE), the latter having recently set the lowest sensitivity limit for observation of the process.

Accomplishments in quark-gluon plasma physics include the discovery of near-perfect liquid behavior and of jet quenching in collisions of gold ions at Brookhaven’s Relativistic Heavy Ion Collider (RHIC). Most recently, the Heavy Flavor Tracker (HFT), constructed at Berkeley, has quantified that heavy quarks lose a large amount of their energy in the plasma similar to the jets. Other notable achievements include producing new forms of antimatter at RHIC (the anti-alpha particle and the anti-hypertriton), possible evidence of the phase transition to quark-gluon plasma in lower energy collisions at RHIC, and measurements of higher temperature plasma properties with heavy-ion collisions in the ALICE (A Large Ion Collider Experiment) detector at the LHC. The study of heavy quarks will continue using the Inner Tracker Upgrade for ALICE, which is currently under construction with Berkeley playing a lead role. Recently, NSD has taken on leadership roles in defining physics goals and detector components for the future Electron-Ion Collider (EIC).

Berkeley Lab has a vibrant program studying nuclear structure, with a focus on the structure of exotic nuclei, especially those with the largest neutron excess or the heaviest masses. Berkeley Lab has a long and distinguished history in developing world-beating detector systems for gamma-ray spectroscopy, and the Lab conceived and built state-of-the-art detector arrays including Gammasphere, currently deployed at ANL, and GRETINA, which recently completed highly successful campaigns involving beams of rare isotopes at NSCL at Michigan State and ANL’s CARIBU facility. This tradition continues with the next-generation Gamma-Ray Energy Tracking Array (GRETA) which has received CD-0 and will have its CD-1 review in 2017.

A strong theory group at Berkeley Lab is actively engaged in building the science cases for the next-generation of advanced nuclear physics facilities to be built in the United States. Notable is work that elucidates the nature of gluonic matter and the structure of the nucleon, which is of great relevance to the next generation Electron-Ion Collider. There is also a growing competency for high-performance computing to study nuclear physics, especially in subfields of quantum chromodynamics on the lattice (lQCD) and nucleosynthesis in supernovae and neutron star collisions.

With respect to quark-gluon plasma (QGP), Lab scientists made seminal measurements showing that the QGP flows with the lowest possible viscosity allowed by the laws of physics. Berkeley Lab’s theoretical and experimental role in discovering the quenching of energetic “jets” was pivotal; the result indicates that the QGP has unprecedentedly high density. The Lab led construction of the ALICE EMCal and DCal, large electromagnetic calorimeters that enable the ALICE experiment to carry out unique jet measurements. Berkeley Lab also led the construction of the STAR Heavy-Flavor Tracker (HFT), a next-generation silicon pixel tracker with unparalleled resolution and thinness, for reconstructing decays of charmed mesons amid the high particle multiplicities at RHIC. Berkeley Lab scientist Howard Wieman received the 2014 Bonner Prize from the American Physical Society to recognize his leadership in developing this and also time projection chamber technologies for environments with high particle
density. HFT results show that heavy charm quark production is quenched, similarly to jets, including charm quarks at relatively high momenta. Berkeley Lab is now leading U.S. participation in an upgrade to the Inner Tracking System (ITS) of ALICE at the LHC, utilizing the technology pioneered for the STAR HFT.

The Lab’s Applied Nuclear Physics program is growing, with applications ranging from nuclear safeguards, radiological monitoring, biomedical applications, and detectors for astrophysics. This work takes advantage of the Lab’s capabilities in innovative instrumentation, including the world-renowned semiconductor laboratory, and attracts many cross-divisional collaborations at the Lab.

The U.S. Nuclear Data Program contributes to the Nuclear Physics program through evaluation and organization of nuclear data for national interests, and is embarking on a series of targeted measurements at Berkeley Lab’s 88-Inch Cyclotron to address gaps in existing data. The 88-Inch Cyclotron supports a local research effort (especially focused on super-heavy nuclei and nuclear data), along with outside users interested in testing electronics and materials for radiation hardness.

LBNL’s Nuclear Physics Core Capability includes innovative equipment and instrumentation, and commensurate handling of big data from experiments that produce multiple petabytes of data per year. Berkeley Lab is leading the development of next generation Electron Cyclotron Resonance (ECR) ion sources essential for next generation accelerator facilities, including FRIB at MSU and the future Electron Ion Collider. At the Sanford Lab in South Dakota, the Majorana Demonstrator is now taking data, utilizing multiple components produced by Berkeley Lab. The Cryogenic Underground Observatory for Rare Events is also taking production data at Gran Sasso in Europe, and the Lab has a strong lead role. GRETINA is producing data, and GRETA is moving ahead. In heavy ion collisions, the Electromagnetic Calorimeter (EMCal) and Di-jet Calorimeter (DCAL) for ALICE, and the high precision, silicon-based STAR HFT were recently completed. Construction is currently underway on several Monolithic Active Pixel Sensor layers for the ALICE inner tracker upgrade. Research is underway to determine how best to apply this novel silicon pixel technology for the sPHENIX experiment at RHIC, and for an eventual Electron Ion Collider detector. The LBNL Semiconductor Detector Lab provides world-class instrumentation for development of advanced germanium and CdZeTe detectors.

Support for this Core Capability is primarily from NP, with contributions from NNSA, ASCR, DoD, and DHS. This capability supports DOE’s missions to understand how quarks and gluons assemble into various forms of matter; how protons and neutrons combine to form atomic nuclei; the fundamental properties of neutrons and neutrinos; and to advance user facilities and instrumentation that reveal the characteristics of nuclear matter.

16. Accelerator Science and Technology

Founded as the first accelerator laboratory, Berkeley Lab has maintained leading capabilities in accelerator development for more than seven decades. The Lab presently has core expertise in the areas of electron and ion sources, magnetic technologies including superconducting magnets, permanent magnets and insertion devices, linear accelerators, synchrotron radiation sources, and laser-plasma acceleration. Through novel upgrades and developments (e.g., superbends, top-off, brightness upgrade), the ALS continues to expand its capabilities and is currently the world’s brightest source of soft X-rays. Investigations are underway for a future facility upgrade that would increase the brightness by up to 3X to produce fully transverse coherent soft-X-ray beams. This would be a cost-effective upgrade, leveraging the investment and existing infrastructure, and will position the ALS as the premier soft x-ray source for decades to come.

Berkeley Lab programs for the development of high-repetition-rate electron sources, advanced FEL design, superconducting undulators, high-brightness electron beam control and manipulations, and laser systems for accelerator applications are coordinated with several other national labs. The Lab leads the world in the developing simulation tools and techniques that model conventional and advanced
accelerators, and the physics of high-intensity laser-matter interaction. This advanced computation is further described in the Computational Science Core Capability.

The Accelerator Science programs greatly enable photon-production systems into the femtosecond and attosecond regime. They are being applied to SLAC’s Linac Coherent Light Source (LCLS) and its successor, LCLS-II. Berkeley Lab is contributing significantly to the new LCLS-II undulators, with expertise derived from our undulator R&D and ALS construction. The Lab is also responsible for principal subsystems of the LCLS-II injector, leveraging expertise gained from the APEX gun, which has recently achieved slice emittance results that are very close to meeting LCLS-II requirements. Further, the Lab has contributed to LCLS-II’s design in the areas of linac systems and accelerator physics.

The ALS remains at the forefront of the technology used for synchrotron light sources, including high-repetition-rate photoinjectors and novel storage-ring designs. The undulator design capabilities, particularly superconducting devices, have the potential to greatly extend the performance of existing synchrotrons, enabling a new suite of fourth-generation facilities that will provide brighter sources at reduced capital and operating costs. This new endeavor benefits from the development of the ultra-high repetition rate electron gun.

Berkeley Lab is the world leader in ultrahigh-gradient laser-driven plasma acceleration technology, producing high-quality GeV electron beams with compact accelerators, a fundamentally new approach for high-energy particle acceleration. The Berkeley Lab Laser Accelerator (BELLA) project, completed in 2012, is enabling laser-plasma acceleration technology in discrete 10 GeV modules using a meter-scale plasma. Experimental campaigns are currently underway to develop the science and technology to reach 10 GeV in a single stage as well as a scaled up version of the staging of two independently powered modules (published in *Nature* in 2016) using BELLA at 5 GeV per module.

The Lab’s Fusion Science and Ion Beam Technology (FS-IBT) Program has significant expertise in developing both ion sources and low-energy beam transport systems and is developing novel accelerator architectures based on micro-electromechanical systems (MEMS) for heating of fusion plasmas and applications in manufacturing. The IBT Group has developed high-yield neutron generators recognized by R&D 100 Awards and is developing neutron based techniques for applications in earth science and carbon monitoring; it has recently extended its research to include gamma-generating devices for national security applications. The group is using the intense, short-ion-beam pulses from the recently completed Neutralized Drift Compression Experiment-II (NDCX-II) to study defect dynamics in solids and has plans to apply intense, short-pulsed ion beams for testing of radiation hardness of electronics for NNSA and DOD. The group also has significant expertise in the formation and doping of highly coherent materials that are used for exploration of concepts for quantum information processing (results appeared in *Nature* in March 2016).

Berkeley Lab has formed a new cross-divisional Berkeley Center for Magnet Technology (BCMT) that covers all areas of magnetic technology: superconducting, permanent, electromagnetic, pulsed and specialty magnets. The primary areas include the superconducting magnet program development of high-field magnets employed in accelerator applications, undulators for light sources and FELs, and specialty magnets for science and applications, as well as fully integrated capabilities from design to manufacturing to testing. The Lab has been involved in the recent successful application that led to the first isolation of a significant mass of antimatter. Future applications will include neutrino science and potentially the development of the next proton or muon collider.

Berkeley Lab is the lead lab for R&D on high field accelerator magnets, with oversight of the DOE-HEP sponsored US Magnet Development Program (MDP). The MDP is a multilab program focused on responding to the P5 report recommendations to develop cost-effective, high performance superconducting accelerator magnets for the next generation of colliders. The program is scoped with
developing cost-effective high field superconducting accelerator magnets requiring little if any training to reach operating parameters, and requiring minimal operating margin for efficient operation.

The Lab’s state-of-the-art superconducting magnet development integrates novel conductors, fabrication and testing. This expertise is being applied across SC programs. Notable examples include the design and fabrication of a superconducting electron-cyclotron resonance source for FRIB, and research on magnet technology utilizing high-temperature superconductors for fusion application. On the international front, Berkeley Lab is a key member of the LHC Accelerator Research Program (LARP) with significant roles in the nascent LHC upgrade project, the HL-LHC AUP, scoped with contributing half of the new interaction-region focusing magnets. LBNL responsibilities include the production of the niobium-tin superconducting cable, procurement of the mechanical structure and final assembly and mechanical loading of the high-field quadrupoles. The alignment of the BCMT with SC priorities is also exemplified in the recent HEP Accelerator Stewardship Program award for developing lighter weight superconducting magnets in gantries to improve patient access to proton or carbon medical therapy.

Supported by HEP and BES, with further sponsorship from FES, ASCR, NE, NNSA, DHS, DoD, ARPA-E, and other federal agencies, this core capability supports SC’s missions to conceive, design and construct scientific user facilities; to probe the properties and dynamics of matter; to advance energy security; and to support DOE’s other scientific discovery and innovation missions.

Applied Science and Energy Technology

17. Applied Materials Science and Engineering.

Berkeley Lab’s research emphasizes the design and synthesis of advanced materials for energy, electronic, structural and other applications in a wide range of physical environments. This capability develops materials that improve the efficiency, economy, environmental acceptability, and safety for applications, including energy generation, conversion, transmission and utilization. Underlying expertise includes nanoscale phenomena, advanced microscopy, physical and mechanical behavior of materials, materials chemistry and biomolecular materials.

Berkeley Lab’s applied materials science and engineering research involves advanced materials and nanotechnology for clean energy, including hydrogen storage and nanostructured organic light-emitting diodes. The Lab has world-leading expertise in the tailoring of the optical properties of window materials, including the characterization of glazing and shading systems, the chromogenics of dynamic glazing materials, and low-emittance coatings for solar performance control. Berkeley Lab also leads the scientific community in the development of plasma-deposition processes to enable improved window coatings.

Berkeley Lab has a strong development program directed toward advanced sensors and sensor materials to control industrial processes to reduce the waste of raw materials on manufacturing lines, increase the energy efficiency of manufacturing processes, and minimize waste. The Lab also studies high-temperature superconductors for electrical transmission cable that could substantially reduce losses during transmission. Capabilities include analyzing the mechanical behavior of novel materials and designing novel materials with enhanced mechanical properties. Berkeley Lab also has extensive expertise in using waste heat for electricity. In addition, the Lab conducts next-generation lithography and supports the development of tools and metrology for size reduction in the next generation of microelectronic chip manufacturing, largely sponsored by industry.

Berkeley Lab focuses software and hardware technology development on novel pathways to sense the grid at unprecedented temporal resolution, systems level integration of automated demand response, and renewables as elements of the next generation grid.
This Core Capability is sponsored by EERE, DHS, ARPA-E and SPP programs, including DoD and industry. It is underpinned by DOE-supported basic chemistry, materials, and computational research, and contributes to DOE missions in energy, the environment and national security. This work benefits DOE technology programs such as solar-energy conversion, electrical-energy storage and transmission, solid-state lighting, energy efficiency and the study of materials in extreme energy environments.

18. Nuclear and Radio Chemistry.

Here, Berkeley Lab’s capabilities include fundamental nuclear measurements; actinide chemistry; the irradiation of electronic components for industry and the government, including post-irradiation and materials characterization; the design, development and deployment of advanced instrumentation; compact neutron and gamma-ray sources for active interrogation; nuclear data management; and substantial modeling and simulation expertise. Work for DOE’s SC includes actinide chemistry with application to chelating agents; for NNSA, advanced detector materials, compact gamma and neutron sources, detection systems and algorithms development, and background data management and analysis. Berkeley Lab’s work for DOE NE through the Spent Fuel and Waste Disposition Campaign (SFWD) includes subsurface modeling and testing to evaluate and improve on the current technical bases for alternative prospective geologic environments for high-level nuclear waste disposal.

Berkeley Lab is a world leader for developing instrumentation that detects and measures ionizing radiation. Radiation-detection materials, including scintillators and solid-state detectors that combine high-density with excellent energy resolution and high-performance electronics for detector read-out. Complete detection and imaging systems are used for a variety of purposes including nuclear medical imaging, nonproliferation and homeland security, as well as fundamental explorations of high-energy and nuclear physics. Unique materials-screening and crystal-growth capabilities enable optimized high-throughput development and design of scintillation- and semiconductor detector materials. Capabilities include large-volume germanium and CdZnTe detector development emphasizing position-sensitive and low-noise systems, gamma-ray imaging using coded aperture masks, and Compton scattering telescopes.

The Air Force and the National Reconnaissance Office support the testing of critical space-based electronic components by the National Security Space Community (NSSC), using heavy-ion beams at the Lab’s 88-Inch Cyclotron. “Cocktail beams,” composed of a mixture of elements that mimic the composition of cosmic rays encountered by satellites, provide a unique national asset to greatly speed the testing of critical space-based electronic components. Other core facilities are the crystal growth facility, BELLA (where compact tunable monochromatic gamma sources are under development for NNSA and DoD), and the Semiconductor Detector Lab.

Berkeley Lab collects high-quality gamma-ray background data in urban and suburban environments with support from DHS. The Lab plans to fully characterize the gamma-ray background based on data collected from detectors in conjunction with visual imagery, light detection and ranging (LIDAR), weather, and other geospatial data that may affect distribution of incident gamma rays. Berkeley Lab is also obtaining and evaluating background gamma-ray data from aerial environments containing complex topographical and isotopic variations. For example, areas of elevated radiation in the contaminated Fukushima region were recently mapped by the novel High-Efficiency Multimode Imager mounted on a remotely controlled helicopter. NNSA supports a feasibility study to explore an advanced system for data storage, analysis and dissemination of gamma-ray background data, including detailed annotation. Standardization and analysis frameworks developed at the Laboratory for the HEP and cosmology communities will vastly increase the scope of the data being analyzed in the future. This Core Capability is sponsored by SC (NP, HEP, and BES), NNSA and NE, as well as DHS, DoD, and the NRC. It contributes to DOE missions to integrate the basic research in SC programs with research in support of NNSA and DOE technology office programs.
19. Systems Engineering and Integration.

Berkeley Lab’s demonstrated abilities to engineer, construct and integrate complex systems underpin many of the core capabilities described in this section, and those of the major user facilities described above. Within DOE’s SC, Berkeley Lab is uniquely configured with a centralized organization that makes engineering, systems and project management, and technical support available to all of the Lab’s scientific endeavors.

Berkeley Lab’s internationally recognized advanced instrumentation skills (e.g., accelerating structures, detectors, data acquisition systems, lasers, magnets and optics) have enabled many of the scientific breakthroughs described in this Plan; these are the direct result of the holistic coordination and deployment of engineering and technical resources. Solutions and approaches developed for one application are routinely leveraged, adapted and applied to others. This disciplined integration and systems approach is a critical part of Berkeley Lab’s contribution to the LCLS-II upgrade, where we are responsible for the injector, undulators and low level RF systems. The Lab also responsibly leads the GRETA, US-CUORE, LUX, DESI and LZ collaborative projects. This approach also underpins the conceptual development of the ALS’s diffraction limited upgrade. Other successfully integrated systems and project management include: the ATLAS inner detector, the GRETINA and ALICE nuclear physics detectors, and the Transmission Electron Aberration-corrected Microscope. Further illustration of this integrating, crosscutting systems approach is Berkeley Lab’s world-leading expertise in integrated silicon detectors for high-energy physics detectors that has been adapted and applied to the development of massive scientific-grade CCD detectors for astronomical applications. This was subsequently adapted and improved to provide radiation-resistant high-speed X-ray and electron detectors. These direct X-ray detecting CCD systems are deployed at national and international light sources.

In addition to Berkeley Lab’s demonstrated abilities to engineer and integrate complex systems for basic science, we are the recognized leader in energy efficiency in commercial and residential buildings and industrial facilities. The Lab develops and transfers new energy-efficient building and industrial technologies from the laboratory to the industrial and commercial world and stimulates the use of high-performance technologies through innovative deployment programs. Berkeley Lab is also a leader in developing cool surface materials for roofing, pavement, and architectural glazing, and in understanding large-scale urban heat-island effects that impact energy consumption and smog formation.

Within the national lab network, Berkeley Lab leads management of transmission reliability programs (CERTS); collaborates with DOE, independent power authorities and states (DRRC); and collaborates with other national labs on energy storage for ancillary services and renewable integration.

In addition to SC, these efforts contribute to technology research programs funded by EERE, FE, EDER, and ARPA-E, as well as the DHS Chemical and Biological Security program. Berkeley Lab leverages DOE’s investment by working with California and other states, and other federal and SPP sponsors, including the Federal Energy Regulatory Commission and the California Energy Commission. The Lab partners with national and international organizations to develop technical standards.

20. Decision Science and Analysis.

Berkeley Lab performs integrated research on energy policies to mitigate carbon emissions and climate change while minimizing externalities such as health burdens, air quality impacts, economic disruptions and water resources impacts. The Lab investigates the economic impact of energy-efficiency performance standards in industrial and commercial building equipment and systems, and for consumer products. The Lab provides technical assistance to federal agencies to: evaluate and deploy renewable, distributed energy, as well as demand-side options to reduce energy costs; manage electric power-grid
stability; and assess the impact of electricity market restructuring, e.g., employing large-scale electric-energy storage systems. Research efforts integrate techno-economic analysis and lifecycle assessment with basic science and technology development to ensure sustainable scale-up.

Berkeley Lab’s role within the lab network is to provide analysis of energy efficiency, clean energy and electricity market policies and standards for energy efficiency requiring complex interconnected technical, economic and environmental analyses. This capability contributes to DOE’s mission by assisting government agencies in developing long-term strategies, policies and programs that encourage energy-efficiency in all sectors and industries. It is sponsored by EERE, OE, FE and NE, as well as the CEC and California Public Utilities Commission (CPUC).


Berkeley Lab’s applied research addresses energy technology design and development, processes, models, networks, systems and energy efficiency. The Lab leads the world in accelerating the transition of battery technology from lab to market (e.g., CalCharge), window technology and performance analysis, modeling of energy saving technologies in building, whole-building and component systems, and evaluating and tracking energy savings in industrial facilities. As a leader in the R&D of battery systems for automotive and stationary applications, Berkeley Lab is a lead partner in the JCESR Hub collaboration. Battery systems research encompasses the development of new materials, theoretical modeling and systems engineering; the Lab also applies its extensive experience in subsurface science to underground compressed-air energy storage. The research in large-scale subsurface energy storage encompasses numerical simulation of coupled processes in the porous reservoir.

The built environment is responsible for 40% of U.S. energy consumption and 70% of U.S. electrical usage; Berkeley Lab performs research on buildings energy efficiency, energy simulation, modeling of whole building systems and components, walls, windows, heating, cooling, ventilation, plug loads, roofing system and refrigeration, as well as analysis and development of control systems, fault diagnostics, measurement and verification, agent based IT, energy information and management systems. Berkeley Lab is also a leader in the research of indoor environmental quality, lighting quality, ventilation and health.

As part of DOE’s grid modernization effort, the Lab advances research on electric grid storage and stationary use, electricity grid modernization through technologies for smart grid, distributed generation (microgrids), energy management and Demand Response, and improved grid reliability. This core capability is sponsored by EERE, OE, ARPA-E, EPA, other federal agencies, the State of California and Utilities. It supports DOE’s mission to develop and deliver market-driven solutions for energy-saving homes, buildings and manufacturing, as well as sustainable transportation.

FLEXLAB, or the Facility for Low Energy eXperiments in buildings, consists of testbeds and simulation platforms for research, development, testing and demonstration of low-energy building technologies, control systems and building systems integration. FLEXLAB maintains a network of industry partners for research, demonstration and deployment. It enables development of cost-effective integrated technology solutions to meet 50% whole-building energy savings — a feat that cannot be met solely by the use of single-component or technology upgrades alone. FLEXLAB’s FY15 budget is $1.06M. Our major sponsors are DOE (BTO, OE), GSA, SCE, PG&E and CEC.


The Lab leads the world in advanced sensing modeling and short-term control in the distribution grid and microgrids. The Lab developed key analytics around grid measurement and Distributed Energy Resources Customer Adoption Model (DER-CAM) for dispatch and the control of microgrids. Berkeley Lab develops hierarchical control schemes and data analysis for large distributions of local power.
generation including solar, storage, electric vehicles to enable multi-level dispatch, and standards development of the interconnection of renewables and smart grid, all to enhance, modernize and support the future distribution grid.

In the National Lab network, Berkeley Lab leads and collaborates within the grid modernization activities, including program management. Collaborators include LLNL, LANL, SNL, ORNL, ANL, SLAC, and PNNL. This core capability contributes to DOE’s efforts to drive electric grid modernization and resiliency in the energy infrastructure, and the development of grid science for a high renewable penetration future. This work at LBNL is supported by EERE-OE, ARPA-E, DoD’s DARPA and ESTCP, and the CEC. The GMLC is a DOE wide activity that is funded by EERE and OE.

Science Strategy for the Future

Berkeley Lab’s enterprise-wide priorities and initiatives are carefully thought-out approaches to extend and support the sciences that are rooted firmly in DOE’s mission needs. The priorities represent enduring commitments that ensure the Lab is able to continue to serve the Department’s mission needs through prudent stewardship of our world-class user facilities and infrastructure, careful visioning of new science support buildings, and well-prepared applications that can leverage next generation computing capabilities as they become available.

The enterprise-wide strategic initiatives explore new scientific directions that leverage Berkeley Lab’s extremely well-integrated programs and facilities, and bring to bear cross-disciplinary expertise and institutional support on critical challenges facing our nation today. These solutions will help the U.S. to continue to maintain scientific leadership in fields critically important to our economic well-being.

Infrastructure

Overview of Site, Facilities and Infrastructure. The Mission Readiness Facilities and Infrastructure Strategy supports Berkeley Lab’s Core Capabilities and meet the Campus Strategy objectives (below) effectively, safely and efficiently. The strategy addresses construction, protection of assets through preventive and corrective maintenance, asset modernization through upgrades and replacements, and demolition of facilities and utilities no longer needed to support DOE’s mission. This section provides an overview of existing infrastructure, and integrates approved and planned investments from DOE, UC and Berkeley Lab to comprise our 10-year infrastructure strategy.

The main Berkeley Lab campus is located adjacent to UC Berkeley, on 202 acres of (UC) land, of which 84 acres are leased to DOE. The site is located within the boundaries of Berkeley and Oakland, California, though local land use restrictions are not applicable to Berkeley Lab. Information on Berkeley Lab land use planning is available in the Berkeley Lab Long-Range Development Plan at http://www.lbl.gov/community/planning/ldrp/.

The main campus structures consist of 1.71 million gross square feet (gsf) of DOE-owned buildings and trailers. Based on updates to the 2015 Laboratory Operations Board (LOB) infrastructure condition assessment, less than 36% of all building assets were ranked as adequate; their average age is 41 years.

There are also 35,672 gsf of UC facilities at the main site, including the domed portion of the ALS, and the UC Guest House.

The utilities infrastructure includes domestic and treated water, low conductivity water, sanitary sewer, storm drain, natural gas, compressed air, electrical, life safety and technology systems (telecommunications, optical fiber, etc.). These systems and their respective components vary greatly in age and condition, reflecting generations of alterations and betterments over Berkeley Lab’s long history. Using the LOB assessment categories and updating to reflect current conditions, 27% of utilities
and site systems as adequate. Significant and ongoing investments in utility systems will be necessary to adequately serve the future needs of science and support operations. A phased replacement strategy, that is coordinated with redevelopment activities, is one way to cost effectively execute large component and branch replacements. Berkeley Lab will use these opportunities to transition towards the use of common utility corridors and modular utility plants (MUPs). Common utility corridors will provide easier access for maintenance and future modifications, lowering lifecycle costs and minimizing disruption of services. MUPs provide an energy-efficient, more redundant and more economical means to meet the chilling and heating loads of building clusters, rather than each building functioning as self-supporting. The generational renewal Berkeley Lab will be experiencing over the next decade provides a unique opportunity for this transition. Taken together, common utility corridors and MUPs will transform Berkeley Lab’s utility infrastructure into a modern, sustainable and cost effective configuration that has become standard among physical plants throughout the world.

Berkeley Lab leases 10 off-site facilities totaling 326,086 gsf for biosciences research (JBEI, ABPDU, KBase, JGI and the Molecular Biophysics and Integrated Bioimaging Division), NERSC (tape libraries) and the Office of the Chief Financial Officer. In FY17 Berkeley Lab is planning to terminate the lease of 2,546 gsf of Livermore Network Operations Center (ESnet) space. In FY20, when IGB is operational, Berkeley Lab is planning to terminate the lease space used to house the JGI and KBase programs. Pursuant to the UC-DOE Prime Contract, Berkeley Lab also has no-fee use of 51,585 gsf of UC space on the UC Berkeley campus.

**Space Utilization Summary for Non-Excess Facilities.** In 2009, Berkeley Lab implemented a utilization assessment program of laboratory, high bay, storage, shops, and support space; in 2013 it added offices to the program. The program’s primary drivers are to identify areas for new or expanding research opportunities and create a lab-wide and transparent data set. Of the ~0.8M gsf assessed, as shown in the table below, ~85% was ranked as fully- or over-utilized; ~15% was ranked as less than fully utilized.

<table>
<thead>
<tr>
<th>Room Category</th>
<th>Repurpose/Reuse</th>
<th>Not Utilized</th>
<th>Under Utilized</th>
<th>Fully Utilized</th>
<th>Over Utilized</th>
<th>TOTAL</th>
</tr>
</thead>
<tbody>
<tr>
<td>HBAY</td>
<td>0</td>
<td>0</td>
<td>4,102</td>
<td>46,666</td>
<td>0</td>
<td>50,768</td>
</tr>
<tr>
<td>LAB</td>
<td>10,216</td>
<td>17,403</td>
<td>15,502</td>
<td>279,828</td>
<td>838</td>
<td>323,787</td>
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<tr>
<td>OFFICE</td>
<td>14,099</td>
<td>18,591</td>
<td>38,856</td>
<td>285,493</td>
<td>314</td>
<td>357,353</td>
</tr>
<tr>
<td>SUPPORT</td>
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<td>781</td>
<td>3,517</td>
<td>612</td>
<td>0</td>
<td>4,910</td>
</tr>
<tr>
<td>STORAGE</td>
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<td>359</td>
<td>777</td>
<td>103,683</td>
<td>0</td>
<td>104,844</td>
</tr>
<tr>
<td>Total</td>
<td>24,340</td>
<td>37,134</td>
<td>62,754</td>
<td>716,282</td>
<td>1,152</td>
<td>841,662</td>
</tr>
</tbody>
</table>

**Overview of 10-year Campus Strategy and Summary of Investments Needed.** Berkeley Lab’s multiyear strategy is based on four objectives that address new facilities construction, existing facilities modernization, utility infrastructure transformation, and the preparation of sites for future development. Taken together, these objectives are intended to transform Berkeley Lab’s aging facilities and infrastructure into a modern, integrated, interactive, sustainable and fully mission-aligned environment for ground-breaking science.

**Objective 1: Construct new facilities to advance research collaborations:** This includes the Integrative Genomics Building (IGB) currently under construction, the proposed Biological and Environmental Program Integration Center (BioEPIC) Building, the proposed State of California and philanthropically funded the Bioenergy and Bioproducts Research Center (BBRC), and other facilities for Biosciences integration, as well as additional Energy Sciences buildings, such as a chemical sciences building and a material sciences laboratory building. These facilities will integrate research programs from dispersed locations onto the former Bevatron and Old Town sites, advance interdisciplinary sciences, further
increase the scientific integration and impacts of the ALS, and vacate leased and seismically deficient buildings.

**Objective 2: Modernize existing facilities for evolving scientific needs:** In anticipation of the planned upgrade of the ALS, the Lab is analyzing its supporting infrastructure for current and future mission readiness. Several projects are under construction or in design to reduce deferred maintenance and improve the infrastructure and utility services to this national user facility including the ALS (B6, B34, B37, B80) HVAC Controls project, replacement of the B37 Cooling Towers, and improvements to the ALS Smoke Evacuation System (as part of FireSAFE). Following completion of this year’s institutional infrastructure assessment and improvement plan, additional infrastructure enhancements will be put forward for prioritization in future years, such as replacing air compressors (at B43) that are beyond useful life, and increasing capacity to address growing demand.

As discussed in Section 4, the **Electron Microscopy Lab-wide Initiative** will enable Berkeley Lab to remain an international electron microscopy powerhouse. An addition to the Molecular Foundry would incorporate a number of synergistic characterization plans across the Lab, which, when combined with the synthesis and theory capabilities at the Foundry, will result in a renewed state-of-the-art, world-leading electron imaging capability for a broad range of users from a diverse set of scientific challenges in areas such as materials synthesis, catalysis, Earth and environmental science, soft matter characterization, and structural biology. Instruments to be developed requiring purpose-built state-of-the-art facilities include ultrafast electron diffraction imaging capabilities; novel *in situ*, time-resolved and cryo-EM instruments, and an analytical TEM with high energy resolution.

HVAC, roofing, utilities and space reconfiguration improvements at the Engineering Division complex (B77 and B77A) are desired to improve production and assembly capabilities in support of several Berkeley Lab programs and DOE complex projects, such as LARP Hi-Lumi, ATLAS, LCLS-II, ALICE, and eventually the planned ALS upgrade. Additional improvements to the institutional infrastructure supporting the BELLA Collaborative Facility (B71) are discussed under gap investments.

As part of the multi-year strategic space consolidation of the Lab’s Earth and Environmental Sciences Area (EESA), modernization and improvements of (B83) are needed to accommodate program growth, provide colocation with other EESA programs, and allow the eventual demolition of B64. This project would address deferred maintenance related to the current HVAC system, improve architectural building elements, and upgrade IT infrastructure. Between this project and the proposed BioEPIC building (which would be half occupied by EESA programs) much of the near and medium term growth currently anticipated in this scientific area could be accommodated.

Replacement and upgrades of the controls and HVAC systems are required at the Advanced Materials Lab (B2), Materials Sciences and Energy Technologies Shared Lab (B66), and Chemical Sciences Lab (B70A), to meet demanding mission-performance requirements for ongoing research that requires equipment sensitive to minor temperature changes and air currents. In the Materials Sciences Lab (B62), the Lab is planning to correct buckling on the first floor and improve the mechanical, life safety, and systems supporting systems. Each of these projects would replace outdated systems, improve space utilization, and significantly reduce deferred maintenance backlogs.

IT Systems require a modular data center unit for new high-density computing systems in support of numerous Berkeley Lab programs. The expected growth in use from every scientific division at the Lab (excluding NERSC) will also require the addition of a second module several years from now and would increase the electrical capacity of 600 kW to 900 kW. The Lab has been forced to turn away government and SPP funded projects requiring additional high performance computing requirement over the previous 18 months due to a lack of capacity to house them. Other long term IT related infrastructure projects are discussed within Objective 3.
While the majority of these projects reduce or avoid growth of Berkeley Lab’s deferred maintenance (DM), the highest priority and mission-critical site-wide DM proposed items in the Infrastructure Investments Enclosure will significantly reduce DM. These proposed projects would rehabilitate HVAC systems, controls, electrical, and other elements within numerous buildings across the site.

Related to the objective of modernizing existing facilities are a subset of projects that would retire high-risk compliance items such as seismic issues, fire alarm upgrades, and security system improvements. These projects are discussed further under the Current Infrastructure Gaps subsection.

Objective 3: Transform utility infrastructure for expansion and reliability: To support new facilities and resolve existing utilities’ deficiencies and relocation requirements, the first phase of a site-wide utility corridor are being developed at the Bayview (former Bevatron) area. This includes proposing site-wide water supply, storm-drain, effluent and hillside stabilization system replacements and repairs to increase service reliability, minimize environmental risk and increase hillside stability. For each of these systems the Lab has ranked branch areas or system components that are of “highest priority” for replacement based on their risk of failure. Critical life safety systems, such as standby power generators and electrical distribution equipment, are proposed for upgrade and replacement to serve load increases, promote reliable emergency service and improve electrical worker safety. Ongoing investments towards mitigating the risks of landslides remain a priority given Berkeley Lab’s topography is dominated by hilly terrain. The proposed FY18 Lab funded Grizzly Peak Substation Switchstation upgrade will allow the Lab to meet increases in electrical peak demand, while maintaining redundant service between its two transformer banks at this, its furthest upstream, substation. Technology infrastructure being considered includes sitewide fiber distribution enhancements, telecommunication room modernization, communication nodes improvements, and WiFi coverage expansion. The majority of these projects will either retire or avoid the growth of DM.

Objective 4: Prepare sites for future development: UC and the Berkeley Lab decided to limit all new construction to brownfield sites; thus, this objective includes demolishing old facilities and cleaning up legacy waste to enable Objective 1 (construction of new facilities), much of which entails the Old Town Demolition Project and Bayview site preparation activities. The former is currently underway and includes the razing of an aging cluster of research buildings and removal of some legacy contamination. The latter is being planned and is discussed further in the Current Infrastructure Gaps subsection.

A campus map (see next page) provides a summary-level overview of the needed infrastructure investments and highlights of our multiyear strategy. This is followed by a discussion of the current and 10-year infrastructure investment gaps of infrastructure support of the Laboratory’s core capabilities. This is followed by details of Berkeley Lab’s 10-year facilities and infrastructure strategy, as well as funding required to achieve the objectives outlined above.

Berkeley Lab Overview and Summary-Level of Needed Investments
Current Infrastructure Gaps

Contamination & External Particle Tunnel Demolition at the Bayview (former Bevatron) site: The IGB project gained CD-3 approval in October 2016 and is currently under construction. Berkeley Lab’s multiyear strategy includes proposing to construct facilities to support full integration of the biosciences programs adjacent to the IGB. These activities are currently dispersed across four off-site locations within a 25-mile radius of the main site. Program integration would enhance biosciences’ synergy, productivity and innovation, and create operational efficiencies over time.

Several areas of VOC-contaminated soil, soil vapor, and groundwater pose a risk to the redevelopment potential of the Bayview site. The extent of VOC-contamination in areas north of the IGB site is unknown and poses a risk to future development activities, such as BioEPIC and BBRC construction. Due to the potentially long lead times required for regulatory interfaces with respect to VOC-contamination clean-up and/or control approaches, it is imperative to begin characterization activities as early as possible. The Lab has started planning for this work with the goal of providing a soil vapor assessment work plan for regulatory review in FY17.

In addition to the previously discussed challenges, demolition of the former Bevatron’s legacy underground External Particle Beam (EPB) Hall utility tunnel and its associated foundation slabs, including any required environmental remediation, will need to be addressed prior to redevelopment. The EPB Hall tunnels and slab removal was outside the scope of the Bevatron Demolition Project. Due to its use as a beamline, the shielding, as well as the concrete walls, floor and roof of the tunnel system must be considered radioactively contaminated material until proven otherwise. Lack of funds to demolish the EPB Hall tunnels and slab could delay full integration of the biosciences programs, and result in increased costs for leased space. Therefore, it is a top priority of the Laboratory to identify the funds needed to complete demolition of the tunnels as early as possible. To this end, the Lab has funded in FY17 an effort to perform a historical assessment and concrete gamma radiation scan/survey of the tunnels. The resulting reports should accelerate the schedule for preparing the site for BioEPIC and allow for stronger cost estimating assumptions. Berkeley Lab is currently researching funding options for addressing these legacy constraints so that it can make use of its largest and most promising development zone.

High Risk Compliance Items: According to the United States Geological Survey, there is a 63% probability of at least one magnitude 6.7 or greater earthquake striking somewhere in the San Francisco Bay region in the next 30 years. Though 17 operational buildings are rated seismically poor, the highest risk of these based on population and functions housed are Health Services (B26), Food Services (B54) and the Fire Department living quarters (B48). The Lab is seeking to retrofit these facilities as early as possible. Additionally, several seismically deficient facilities are planned for demolition as soon as funding can be made available including B50C, B58A, B70, B73, and B73A. Several other seismically-deficient buildings are also slated for demolition over the next decade and are discussed in the Future (10 years) Infrastructure Gaps subsection.

The Fire and Safety Alarm Future Enhancements (Fire SAFE) Project is a plan to replace and upgrade the existing fire and safety alarm systems. The plan is sequenced over a funding-dependent, multi-year period based upon building risks, operational priorities and the condition of the existing systems. Objectives include: replacement of fire alarm control panels and connected devices, the majority of which are controlled by panels that will reach end-of life in 2017; identify and connect existing and new safety detection and alarm devices (e.g., toxic gas, oxygen depletion, etc.) to a life safety system; and upgrade existing buildings to current life safety standards including mass notification system, horn/strobe lights for the hearing impaired, exterior building strobes and moving message signs, and placement of manual pull stations to meet Americans with Disabilities Act requirements. FireSAFE ensures continued compliance with applicable building codes, fire codes and DOE Orders; it increases
the protection to personnel and assets through early detection and notification of fire and life/safety events.

The Building Perimeter Protection project will improve personnel and property protection in Lab buildings to ensure compliance with the 2016 Site Security Plan and emerging DOE requirements. At present, the Lab lacks the ability to remotely lock all exterior doors in the event of an active shooter or other significant security event. This multi-year effort will extend the access control system’s reach by installing access control equipment on exterior building doors and adding intrusion detection devices in areas housing high risk operations or equipment. Improvements will be completed on a building-by-building schedule based on each building’s risk level, addressing the riskiest buildings first. Project timeline is dependent upon funding availability, operational priorities, and the complexity of retrofitting buildings constructed in many different ways. The Building Perimeter Project will improve personal safety for Lab workers, visitors and security patrol officers, exclude external threats from building entry remotely, and ensure compliance with anticipated DOE and contract requirements.

The Video Surveillance Replacement Project provides video capabilities essential to controlling the increases in security personnel costs and providing affordable protection of Lab personnel and DOE assets. This will meet the Lab’s need for improved situational awareness and remote visibility of high-value/high-consequence locations, and provide high quality detection of potential security threats without costly human surveillance. The Lab’s small current video installation is past the end of its useful life, lacks video analytics capability, and is not integrated with alarm monitoring. Field security officers must go to the location of alarms and complaints to assess the severity and source of threats, exposing them to potential harm from active shooters or toxic substance releases. This project will build a stable and expandable framework that complements and integrates with other security operations improvements to affordably manage the Lab’s potential threats.

The Employee Gate Authenticated Entry Project will significantly reduce the risk of inappropriate site entry, improve compliance with the Site Security Plan, and decrease security expenses by providing the technology needed to institute authenticated access control at the Lab’s three main gates. The project will improve security system capabilities and implement new entry procedures to automate authentication and access processes for employees.

Future (10 years) Infrastructure Gaps

Replace the ALS Support Building: The ALS is a global center for soft X-ray science and innovation for DOE. As such, ALS’s facilities should provide researchers with unique opportunities to interact on the theoretical and experimental facets of photon science. The Old Town Demolition Project currently underway will raze the aging cluster of research buildings that are adjacent to the ALS, remove legacy contamination, and prepare a two-acre site for productive reuse.

Berkeley Lab is planning to consolidate centers for the Materials and Chemical Sciences Divisions, and also potentially extend beamlines from the ALS where B7 (ALS Support Bldg.) is located. A current Investment Gap identified in the Infrastructure Investments Enclosure is the replacement of B7 in an alternate location strategically placed and custom configured to improve support functions. This is a Lab priority to improve and expand this critical support function.

Additional Grizzly Substation Transformer Bank: The main Grizzly Peak Substation is currently configured with two 41MW transformer banks (with functional capacities of 32.8MW) either of which can provide Berkeley Lab’s full electrical power demand. This configuration provides the ability to perform routine and unplanned maintenance on one transformer bank while the Laboratory remains fully operational on the other.
Shyh Wang Hall provides the NERSC HPC program with electrical energy at ~60% the cost of their former location in Oakland. The program is expecting new generations of NERSC high-performance computers to come on-line in 2020 and 2024. The current power load projections, inclusive of NERSC and sitewide incremental power increases, may exceed the functional capacity of each existing transformer banks in either 2020 or 2024. When these projections are realized, an additional transformer bank will be required at the Grizzly Peak Substation to maintain the existing maintenance capabilities. Without the additional transformer bank, the Lab could experience research program load curtailments for every routine and unplanned maintenance event. Even if NERSC’s HPC projections are not realized in the near term, the Lab’s ability to host exciting new project and program opportunities will be significantly constrained moving forward if enhancements to the existing electrical distribution infrastructure are not made. Therefore, to remain competitive, it’s strategically essential to make this investment, and others over the longer term.

Demolition of Seismically-Deficient Buildings: Berkeley Lab’s facility and infrastructure Objective 1 includes facilities for biosciences integration, as well as joint physical, energy science and technology collaborations. To achieve this objective, several seismically deficient lab and research office buildings (55, 56, 60, 63, and 64) must be vacated and demolished.

B70 must also be vacated and demolished due to its inadequate condition assessment and poor seismic ratings. Its occupants would need to be dispersed across the site, including the facilities proposed for the Old Town Site. Buildings 73 and 73A are unusable due to severe seismic deficiencies. Trailers 31A, and 75E are significantly beyond their useful lives and their sites could be used much more effectively. The same is true of environmental monitoring station 13B. These assets were constructed under 1940’s–1970’s building codes and estimates indicate it is not cost-effective to retrofit them. Safe and mission-capable research space is fundamental to DOE’s challenging scientific mission objectives. Recent engineering evaluations have identified both significant and extensive seismic safety hazards in these buildings that will fail during the predicted magnitude-7.0+ earthquake on the Hayward Fault or a magnitude-8.3+ earthquake on the San Andreas Fault. Berkeley Lab proposes to vacate those currently occupied and demolish these buildings to eliminate seismic risks, and prepare the sites for productive re-use.

Berkeley Center for Magnet Technology (BCMT). Many of the Lab’s science programs involve experiments and facilities operating at cryogenic temperatures; these require a Helium liquefier, or an upgrade to the present equipment. The HEP-funded Superconducting Magnet Program (SMP) within the BCMT is one such facility. SMP has made recent investments to improve Helium gas recovery and storage, but the liquefier itself is antiquated and its performance no longer satisfies program needs. BCMT management has developed a plan for a cryoplant upgrade that can leverage the prior He storage investments while satisfying broader LHe needs. The plan’s most critical element is the procurement of a new liquefier, which would provide liquid directly to the magnet test facility and provide liquid in transportable dewars to other users. The procurement would include associated elements such as LHe storage dewars and piping for gas recovery from experimental users at the ALS and Materials Science (Buildings 6 and 2). The Engineering Division would run the cryoplant facility and support science programs within ATAP, ALS, MSD and others.

Building 71 Mechanical System Upgrades. B71 Mechanical System Upgrades would provide the utility infrastructure necessary for the operation of a proposed new beamline with multi-program benefits. The utility infrastructure would upgrade the existing mechanical system capabilities to support the planned use of a short focal length beamline as an extension of the existing BELLA petawatt laser. Sources of funding are being investigated.
**Building 71 Experimental Cave Infrastructure.** The B71 Experimental Cave Infrastructure would provide utility infrastructure to support the installation of a high average power laser system to enable high repetition rate applications of laser plasma accelerators.

**Deferred Maintenance**

The deferred maintenance trend forecast for 2017 will decrease by approximately $5M to $262M and continue trending lower throughout the planning period. Increased investment in DM reduction by the Lab will provide the means for a decreasing DM trend during this period. If the plan described in these pages is implemented as proposed, the projected year 2027 deferred maintenance value would be reduced to the $36M stated herein.
Lab-at-a-Glance

**Location:** Oak Ridge, TN  
**Type:** Multi-program Laboratory  
**Contractor:** UT-Battelle, LLC  
**Site Office:** ORNL Site Office  
**Website:** [www.ornl.gov](http://www.ornl.gov)

### Physical Assets:
- 4,421 acres and 250 buildings  
- 4.8 million GSF in buildings  
- Replacement Plant Value: $6.5B  
- 1.5M GSF in 67 Excess Facilities  
- 1M GSF in Leased Facilities

### Human Capital:
- 4,983 Full Time Equivalent Employees (FTEs)  
- 192 Joint Faculty  
- 305 Postdoctoral Researchers  
- 317 Graduate Students  
- 294 Undergraduate Students  
- 3,131 Facility Users  
- 1,763 Visiting Scientists

### Mission Overview

The mission of Oak Ridge National Laboratory (ORNL) is to be a world leader in transformational scientific discoveries and disruptive technological innovations, with a focus on delivering solutions for clean energy, global security, and economic benefits to the U.S. economy. ORNL’s unparalleled science and technology capabilities are a vital asset within the national research enterprise, enabling science breakthroughs and addressing challenges faced by the U.S. Department of Energy (DOE), other sponsors, and the nation.

Established in 1943 as part of the Manhattan Project, ORNL’s original mission was the production and separation of plutonium. After World War II, ORNL led early work on nuclear energy, radioisotopes for medicine, and effects of radiation on materials and biological systems.

ORNL is home to top-notch talent, facilities, and programs, and is a world leader in materials, neutron, and nuclear science and engineering, and in high-performance computing and data analytics. These strengths along with other multidisciplinary capabilities are deployed, often in combination, in support of a wide range of programs. ORNL has a track record of project management and currently manages the Exascale Computing and US ITER projects for DOE.
ORNL is renowned for its world class, large scale user facilities that are open to the broad science and engineering community. The Spallation Neutron Source and High Flux Isotope Reactor offer unmatched capabilities for understanding structure and dynamics, and robust plans for upgrades will sustain U.S. leadership. The Center for Nanophase Materials Sciences is home to instrumentation and expertise for imaging, fabrication, and characterization at the nanoscale. World-leading computers, Titan and Summit, are principal elements of the Oak Ridge Leadership Computing Facility. Unique facilities that support collaborative work include the Manufacturing Demonstration Facility and those for materials separations and characterization in a nuclear environment.

ORNL has a history and culture of solving “hard problems” with national scope and impact. Research carried out at the Laboratory—from fundamental to ready-to-transition— has advanced science and technology in areas that are improving energy production, national security, human health, and environment, and has led to innovations that are creating new products, new businesses, and new jobs.

Core Capabilities

Of the 24 core capabilities distributed across DOE’s national laboratories, ORNL possesses 23, indicating the exceptional breadth of its scientific and technological foundation. Each comprises a substantial combination of people, equipment, and facilities having unique or world-leading components. Synergies among these core capabilities enable scientific discovery and translational research to accelerate the delivery of technology solutions. The core capabilities are employed in mission delivery for DOE, the National Nuclear Security Administration (NNSA), the US Department of Homeland Security (DHS), and other sponsors.

The application of ORNL’s core capabilities to the needs of non-DOE sponsors through Strategic Partnership Projects (SPPs) and other mechanisms, detailed in Section 5 and Appendix A, ensures the fullest use of DOE’s investment in research and development (R&D). At the same time, non-DOE-sponsored research strengthens ORNL’s core capabilities and enhances the Laboratory’s ability to deliver on DOE’s missions.

To sustain and extend our core capabilities, we continue to invest in our scientific and technical staff, supporting them in building productive careers in R&D, and challenging ourselves, individually and collectively, to be a premier research organization.

The Laboratory’s 23 core capabilities provide a broad S&T base that will lead to fundamental scientific advances and breakthroughs and that will support achievement of DOE missions broadly. This combination of exceptional people, equipment, and facilities will allow ORNL to respond to changing priorities, and to focus on critical needs of the nation.

1. Accelerator Science and Technology

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<th>ORNL core capabilities</th>
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<td>- Accelerator Science and Technology</td>
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<td>- Power Systems and Electrical Engineering</td>
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<td>- Systems Engineering and Integration</td>
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ORNL has world-leading expertise in the basic physics of high-intensity beams and the technology to support production, acceleration, accumulation, and utilization of such high-intensity, high-power beams. The Spallation Neutron Source (SNS) accelerator complex, operating at ≥1 MW beam power on target, is the world’s most powerful pulsed-proton accelerator and the world’s sole superconducting linear accelerator for hadrons. The SNS enables ORNL to lead investigation of the dynamics of high-intensity hadron beams and the development of high-power proton targets.

Other ORNL leadership areas include expertise in negative hydrogen ion sources and low-energy beam chopping and manipulation; superconducting radio-frequency (RF) technology; high-power target systems; high-power and low-level RF systems; pulsed-power technology; sophisticated control systems for the manipulation of high-power beams; beam-tuning algorithms; high-level real-time accelerator modeling and analysis; and instrumentation to measure properties of high-intensity, high-power hadron beams. In addition, ORNL’s strengths in computational science are used to develop beam dynamics modeling and data management tools to design next-generation spallation neutron sources, high-intensity linear accelerators (linacs), and storage rings. The combination of state-of-the-art beam dynamics modeling tools and access to robust experimental data on collective, halo-formation, and instability effects in high-intensity hadron linacs and accumulator rings is unique to ORNL. These strengths underpin our efforts to systematically increase the power level at which SNS operates reliably.

The comprehensive Cryogenic Test Facility supports a robust research program that has led to the development and successful deployment of a novel in situ plasma-cleaning technology that has increased the peak gradients of selected superconducting high-beta accelerator cavities by up to 25%. ORNL is transferring this technology to other important accelerator projects in the DOE portfolio. ORNL is also developing capabilities for laser-based stripping of energetic H– ions to facilitate high-power beam injection into advanced rings, pursuing novel approaches to power conversion technology for klystron modulators, and developing advanced beam instrumentation systems. Continued advances in high-level real-time applications, in combination with improvements in warm accelerator structure vacuum systems, have led to significant reduction in the time required to complete facility turn-on after long outages.

ORNL has constructed and commissioned a low-energy Beam Test Facility. The spare RF quadrupole (RFQ) structure has been commissioned to full power, and a robust program of scientific study is under way that will characterize, for the first time, the full six-dimensional phase space of a low-energy hadron beam. Future research will focus on understanding the formation of beam halo in high-intensity hadron accelerators as well as developing novel neutron moderator technologies. The SNS accelerator complex, in combination with the Cryogenic Test Facility and the Beam Test Facility, provides an essential resource to attract, engage, and retain staff with the expertise to drive innovation in all facets of accelerator science and technology relevant to the ORNL mission.

The impact of ORNL’s research in high-intensity beam dynamics and technology spans all fields of science enabled by high-power hadron accelerators. ORNL staff members are strongly engaged with similar international accelerator facilities as reviewers and advisors. DOE’s Office of Science (SC) is the primary source of funding [mission areas SC-10, 30]; additional support is provided through partnerships with the University of Tennessee (UT) funded by SC’s High-Energy Physics (HEP) program and the National Science Foundation (NSF).

The SC Basic Energy Science (BES) program [mission area SC-10] and Nuclear Physics (NP) program [mission areas SC-25, 30] are the primary sources of funding for the ongoing accelerator S&T activities.

Advanced Computer Science, Visualization, and Data

ORNL’s scientists develop tools and system software for leadership-class computers and applications (e.g., ADIOS, Aspen, Oxbow, Hercules, OpenARC) that are used to address problems of national
importance. In addition, ORNL develops visual analytics tools to support scientific visualization of data and information (e.g., EVAL, Eden, Origami) for use with the Exploratory Visualization Environment for Research in Science and Technology (EVEREST), the Compute and Data Environment for Science (CADES), and the Oak Ridge Leadership Computing Facility (OLCF). ORNL enables translation from R&D to deployment through collocated, integrated expertise in scalable system software, component technologies, architecture-aware algorithms, virtualization, and real-time large-scale data analytics for exascale and advanced computing.

ORNL also enables scientific discovery and accelerates deployment of advanced technologies in energy and national security by developing, managing, and accessing scientific data repositories [e.g., the Atmospheric Radiation Measurement (ARM) Data Archive, Carbon Dioxide Information Analysis Center, Distributed Active Archive Center (DAAC), Earth System Grid Federation, National Extreme Events Data and Research Center, A Large Ion Collider Experiment (ALICE) USA Tier 2]. Through software and architectural advances such as quantum and neuromorphic computing for next-generation architectures, ORNL accelerates the deployment and utilization of petascale- and exascale-capable systems. These R&D activities will deliver exascale-capable systems that will contribute to solving critical national challenges in science, energy assurance, national security, advanced manufacturing, and health care.

ORNL is a leader in predictive performance and future-generation high-end computing architectures. Researchers have significant expertise in system software, component technologies, run time optimization, architecture-aware algorithms, resilient computations, and networking. This expertise is applied to improve the performance, efficiency, reliability, and usability of extreme-scale architectures and to execute large-scale high-performance computing (HPC) science and engineering applications. Researchers in computer science and mathematics focus on computational code performance improvement (e.g., testing and developing tools, libraries, languages).

The HPC resources of OLCF, including the Cray XK7 Titan, are available to users to advance knowledge in areas such as designing fusion reactors, designing new materials, engineering proteins to treat diseases, efficiently releasing energy from biomass, and understanding climate change impact. In addition, the Cray XT6-HE Gaea system is operated for the National Climate-Computing Research Center of the National Oceanic and Atmospheric Administration (NOAA), facilitating multi agency cooperation and R&D partnerships across the climate research community. CADES, launched internally to provide a fully integrated infrastructure offering compute and data services for researchers, is now being applied to the needs of external users, including the National Library of Medicine. With this platform, researchers can process, manage, and analyze large amounts of data using scalable storage, data analysis, and visualization tools. ORNL is home to the Extreme-Scale Systems Center, a national center of excellence in HPC architecture, software, and data analytics funded by the US Department of Defense (DoD), and maintains the nation’s chemical security database and vulnerability modeling capability, funded by DHS. The availability of forefront HPC resources on the ORNL campus also supports the Urban Dynamics Institute (UDI), the Institute for Functional Imaging of Materials (IFIM), the Health Data Sciences Institute (HDSI), and the Consortium for the Advanced Simulation of Light Water Reactors (CASL).

ORNL is committed to growing the nation’s expertise in data analytics and visualization through a joint Data Science and Engineering Ph.D. program with UT within the Bredesen Center for Interdisciplinary Research and Graduate Education. This capability is supported by SC [mission areas SC-1–8, 12, 13, 16], DOE’s Office of Electricity Delivery and Energy Reliability (OE) [mission area ES-10], and SPP customers including DHS, US Intelligence Community (IC), DoD, and US Department of Health and Human Services (DHHS).
2. Applied Materials Science and Engineering

ORNL possesses world-leading expertise in experimental, theoretical, and computational materials research and strongly couples a world-leading fundamental condensed matter and materials science program funded by BES (see Sect. 3.11) to the development of new materials for energy and national security applications. Our applied materials program focuses on developing new materials for optimized performance, especially in extreme environments. As part of the Critical Materials Institute (CMI), a family of Al-Ce alloys have been developed that open the door for more lightweight, fuel-efficient vehicles. A further, ORNL has exceptionally broad capabilities for the design, synthesis, prediction, and characterization of materials with specified structure-property relationships and for understanding the role of defects in controlling materials properties and performance. This core capability supports the development of materials that improve efficiency, economy, and safety in energy generation, conversion, transmission, and end-use technologies.

A distinguishing characteristic of applied materials science research at ORNL is the close coupling of basic and applied research to develop next-generation structural materials for applications in fission and fusion energy, transportation, buildings, high-efficiency steam generation, and advanced power cycles utilizing supercritical CO\textsubscript{2}. Research in this core capability is particularly relevant to manufacturing and a source of the majority of ORNL’s patents. Novel processing techniques for manufacturing include additive manufacturing of metals, alloys, and polymer composites. For example, ORNL demonstrated, for the first time, site-specific texture control during electron-beam powder-bed deposition of a Ti alloy. Specialized capabilities in applied materials science and engineering include materials joining, surface engineering and processing, corrosion studies under harsh but well-controlled conditions, mechanical testing in a variety of environments, and physical property determination. Specific materials expertise exists in advanced alloys, ceramics, nanomaterials, carbon fiber and composites, nanostructured carbons, polymers, energy storage materials (including batteries and supercapacitors), photovoltaics, and thermoelectrics. Outstanding examples of alloy development/qualification are the clad and insulation materials used in radioisotope thermoelectric generators that power the National Aeronautics and Space Administration’s (NASA) deep space probes, including New Horizons, and the recent discovery of a new family of cast Al alloys with greater strength at higher temperatures than those currently used (US patent applied for).

ORNL’s applied materials science and engineering program takes advantage of ORNL’s state-of-the-art capabilities for materials development and testing: SC user facilities, such as the Center for Nanophase Materials Sciences (CNMS), SNS, High Flux Isotope Reactor (HFIR), and OLCF; the Carbon Fiber Technology Facility (CFTF) and Manufacturing Demonstration Facility (MDF) supported by DOE’s Office of Energy Efficiency and Renewable Energy (EERE); and other facilities, such as the Low Activation Materials Design and Analysis (LAMDA) laboratories, and the Irradiated Materials Examination and Testing hot cell facility. Examining materials behavior at extremes is enabled by specialized ORNL facilities and equipment offering access to high temperatures, high pressures, neutron irradiation, and intense magnetic fields, coupled with testing capabilities that range from basic fracture mechanics to a modern creep testing facility to friction and wear.

Strong industrial interactions and technology transfer result in substantial impacts on materials production and utilization, with benefits for efficient production, transmission and use. An example is the development of a nanoporous glass-based coating with graded refractive index characteristics that

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4 Z. Sims et al., *JOM* 68, 1940 (2016)
enable water-repellency and suppression of Fresnel reflections from glass surfaces; this coating has been licensed to Samsung.6

Funding comes from EERE [mission areas ES-2, 4, 5, 8, 10, 13, 14, 15], DOE Office of Fossil Energy (FE) [mission areas FE-3, 4], DOE Office of Nuclear Energy (NE) [mission areas NE-1–3], NNSA [mission areas NNSA-1–3], DHS [mission area HS-9], DOE Advanced Research Projects Agency-Energy (ARPA-E), DoD, and other SPP customers.

3. Applied Mathematics

ORNL’s applied mathematics capability includes extensive expertise in the development, approximation, and analysis of innovative, massively scalable, and resilient mathematical and computational approaches for scientific (model) discovery as well as decision-sciences. ORNL researchers are developing extreme-scale, architecture-aware, and resilient mathematical and computational approaches to take advantage of and realize the potential of future computing platforms, including exascale. The broad scope of research and development of ORNL’s applied mathematics program encapsulate both theoretical and numerical solutions of complex deterministic and stochastic systems, for their immediate impact on a number of applications sponsored by SC’s Fusion Energy Science (FES), HEP, Basic Energy Research (BER), BES and NP.

Two of the more visible projects associated with the applied mathematics program at ORNL are ACUMEN (ACcurate qUantified Mathematical mEthods for Neutron and experimental science) and EQUINOX (Environment for Quantifying Uncertainty: Integrated aNd Optimized at the eXtreme-scale). These projects represent: (1) fundamental research in mathematics, statistics, and computational science for a diverse set of applications of national interest; (2) our impact on the sophisticated experimental and computational DOE and international facilities; and (3) our commitment to interface the frontiers of science and education by actively engaging the applied mathematics community through leading events to rapidly disseminate scientific advances in highest caliber journals, conferences, and workshops.

ACUMEN is a partnership between ORNL mathematicians and instrument scientists at SNS, HFIR, and CNMS to develop and deploy innovative methods to address the challenges faced by experimental scientists. ACUMEN impact includes: several publications in Nature Materials and SIAM Imaging; citations in the annual report from SNS; the organization of multidisciplinary workshops; and delivery of high-performance computing codes that are supported through the workflow Bellerophon Environment for Analysis of Materials (BEAM).

EQUINOX addresses the fundamental question: "how do the uncertainties ubiquitous in all modeling efforts affect our predictions and understanding of complex phenomena?" The primary scientific achievement of EQUINOX is delivery and deploy of a unified and massively scalable computational Toolkit for Adaptive Stochastic Modeling and Non-Intrusive ApproximatioN (TASMANIAN). TASMANIAN represents an architecture-aware, predictive capability for applications that dominate the focus of the DOE mission. ORNL has also co-developed the ensemble propagation techniques at the scalar level of the simulation through the Stokhos package in Trilinos, and integrated within the Kokkos package for many-core performance portability, allowing this technique to be applied in a portable manner to existing CPU, GPU, and accelerator architectures. Additional accomplishments include: numerous international awards and honors; invited plenary talks, chairing international conferences; and significant publications in the highest impact mathematics journals and books including Acta Numerica,

SIAM Review, Numerishe Mathematik, and SIAM Journals on Numerical Analysis, Computational Science, and Uncertainty Quantification.

ORNL provides leadership in the areas of uncertainty quantification, optimization, and control of high-dimensional physical and engineering systems; linear and nonlinear solvers; optimal reconstruction from both sparse and extensive noisy data; advanced methods for multiphysics/multiscale local and nonlocal problems as well as network problems. ORNL’s applied mathematics program also specializes in: numerical algorithms in linear algebra; massively scalable and resilient programming models; the use of advanced-computer architectures; and tools for highly heterogeneous parallel computers. ORNL supports the development and maintenance of high quality mathematical software, including: TASMANIAN, EISPACK; LINPACK; BLAS; LAPACK; ScaLAPACK; Netlib; PVM; MPI; NetSolve; Top500; ATLAS; and PAPI.

Funding comes primarily from SC [mission areas SC-1, 2, 8, 13], DoD, NSF, DHHS, and other SPP sponsors.

4. Biological and Bioprocess Engineering

ORNL brings substantial strength in fundamental biology to bioprocessing and bioengineering to address DOE missions in bioenergy production, carbon biosequestration, and environmental contaminants processing. ORNL is (1) leading the BioEnergy Science Center (BESC), a nexus for research on biomass utilization for advanced biofuels and products (e.g., higher alcohols, esters, and lignin coproducts); (2) characterizing the largest population of Populus genotypes for biomass deconstruction gene discovery; (3) developing new microbial platforms for the control of biomass deconstruction and global carbon cycles; (4) coupling fundamental and applied research in biomass production and conversion for applications in materials and advanced combustion; and (5) making sustained contributions to bioenergy feedstock resource assessment and supply projections.

ORNL leverages its broad capabilities in chemical engineering, materials science, and systems engineering to accelerate translation of research outcomes into demonstrable improvements in bioproducts and biofuels, and to move bioremediation research from the lab to the field or pilot level. Integrated teams at ORNL bridge science to applications. For example, ORNL recently licensed technology to reduce lignin content and recalcitrance in biofuels crops and forage crops (licensed to two companies). ORNL uses expertise in plant sciences, microbiology, molecular biology, and bioinformatics, in combination with facilities such as the common gardens and the ORNL computing resources (CADES, OLCF), to address bioproduct and biofuels production and carbon sequestration. ORNL applies materials and chemical sciences capabilities to develop corrosion-resistant materials for use in bioprocessing systems, and to improve microbial fuel cells, improve carbon fiber production at CFTF, and produce bionanomaterials such as nanomaterials for use in light-emitting diodes and radar-reflecting coatings.

ORNL is a recognized leader in multiple aspects of bioenergy production, including biofeedstock sources and sustainability analyses, with emphasis on an integrated systems approach (e.g., landscape design) at multiple landscape scales (from hectare to nation) for applied impacts. This leadership has been leveraged in the development of the “Billion Ton” studies and of sustainability metrics and analysis, including those for water impacts. ORNL also leads in the use of a suite of biomass conversion processes: novel microbes and applied systems biology, pyrolysis modeling, and biofuels and bioproduct upgrading to advance bioenergy production. Building on identification of key genes that can be manipulated to improve bioprocessing for fuel and co-product production, ORNL has developed innovations resulting in patents and licenses (e.g., C5 FUELTM).

ORNL user facilities including SNS, HFIR, OLCF, and the National Transportation Research Center (NTRC), along with the UT-ORNL Joint Institute for Biological Sciences (JIBS), greenhouse facilities, and CADES provide the needed infrastructure to accelerate discovery and technology development. SC [mission
areas SC-12, 15] and EERE [mission area ES-8] are the primary sponsors of this work. ORNL also performs impact analyses for the US Environmental Protection Agency (EPA) and bioremediation design projects for DoD. Other current sponsors include the National Institutes of Health (NIH), the US Department of Agriculture, and ARPA-E.

5. Biological Systems Science

ORNL’s core capability in biological systems science directly improves understanding of complex biological systems through (1) integration of plant sciences, synthetic biology, ecology, computational biology, imaging, and microbiology; (2) discovery of gene function; (3) foundational research in plant science that enables development of sustainable plant feedstocks for bioenergy and bio-derived materials; (4) modeling of molecular dynamics of proteins; and (5) development of adaptive imaging at multiple spatial and temporal scales. The fundamental understanding delivered through application of this core capability is essential to the solution of challenging societal problems in bioenergy, nutrient cycling, climate change, carbon management, and environmental remediation. For example, ORNL is the host institution for BESC, which has a strong record of research that is leading to demonstrable improvements in the economics and sustainable production of biomass and its conversion to bio-products and bio-materials, such as advanced biofuels and carbon fiber. Fundamental research performed by BESC is rapidly advancing the understanding of cell wall structure and plant feedstock systems. ORNL leads a team that has proposed the Center of Bioenergy Innovation (CBI) as a successor to BESC with a shift in focus to sustainability and a more diverse set of bio-derived materials and advanced fuels.

Within the framework of the Science Focus Areas (SFAs) established by SC’s Biological and Environmental Research (BER) Program, ORNL is expanding research on biocomplexity to facilitate understanding of the structural organization, functional dynamics, and emergent properties that underlie molecular transport, metabolism, compartmentalization, and signaling within and between cells, whole organisms, and their physical and chemical environment. ORNL research on plant-microbe interfaces characterizes the soil and plant microbiome and examines fundamental aspects of plant-microbe signaling and beneficial associations to predict carbon sequestration in the terrestrial biosphere, predict ecosystem response to climate change, and increase sustainability. These data-rich experimental efforts interface with bio-informatics expertise in microbial annotation and in construction and interpretation of complex systems biology data.

ORNL has strategic strengths in plant biology that have largely focused on Populus, in part through a series of highly successful genome-wide association studies focusing on unique genetic resource of more than 1000 genome-sequenced Populus lines in common gardens. ORNL is working in conjunction with Dr. Thomas Juenger (University of Texas) to develop a similar resource for switchgrass. ORNL has demonstrated that these resources allow for efficient identification of gene functions by measurement of phenotypes tied to precise genome-wide association studies. ORNL plans to add to these capabilities by purchasing a state-of-the-art multi-spectral imaging system for phenotyping.

Biological systems science at ORNL also focuses on the biological transformations of critical DOE-relevant pollutants such as mercury, nutrients, and carbon. Capabilities in biomass, neutrons, and computing are combined in the Biofuels SFA. ORNL is applying nanoscale, multimodal spectroscopic, and neutron imaging to plant-microbe interfaces research in newly developing projects. Additionally, ORNL partners with other national laboratories on BER projects such as the Ecosystems and Networks Integrated with Genes and Molecular Assemblies (ENIGMA) consortium and the Systems Biology Knowledge base (KBase).

ORNL’s unique resources include the Center for Structural Molecular Biology (CSMB), the Biological Small-Angle Neutron Scattering (Bio-SANS) instrument at HFIR, and specialized mass spectrometry.
instruments and expertise. CSMB takes advantage of specialized facilities for sample deuteration, neutron scattering, and HPC. Research in this core capability uses SNS, OLCF, CADES, JIBS, and state-of-the-art greenhouses, environmental chambers, and characterization laboratories.

SC [mission areas SC-4, 12–16] and EERE [mission areas ES-2, 8, 13] are the primary sponsors of the work within this capability. Additional work is sponsored by DHS [mission area HS-3], NIH, ARPA-E, DoD, and EPA.

6. Chemical Engineering

ORNL’s capabilities in chemical engineering span discovery and applied research. These capabilities leverage core capabilities in chemical and molecular science, nuclear chemistry and radiochemistry, condensed matter physics and materials sciences, applied materials sciences and engineering, biological and bioprocessing science, and computational science. Leadership in chemical separations, catalysis, isotope production, high-efficiency clean combustion, and biofuel production enables ORNL to develop new chemical processes and separations technologies that improve efficiency, economy, environmental acceptability, and safety in energy generation, conversion, and utilization. For example, a new non-noble-metal, low-temperature emission control catalyst was developed for oxidation of carbon monoxide without inhibition from hydrocarbons. This development could reduce the emissions from lean-burning diesel engines and reduce the cost for emission catalysts. Research in isotope production and separation, environmental remediation, and actinide separations is also underpinned by this capability.

Technology development through chemical engineering often builds directly on (1) BES-sponsored fundamental research in materials design, synthesis, and characterization; (2) BES-sponsored research in chemical separations, catalysis, and computational modeling; (3) BER-sponsored research in bio-based fuels and chemical production; (4) NP-sponsored research in isotope production; and (5) EERE Vehicle Technologies Office and Bioenergy Technologies Office-sponsored research in applied chemical separations, fuels, pyrolysis, and catalysis development. Example results include new polymeric materials to extract uranium from seawater and novel materials to separate and capture CO2. This capability also enables ORNL to develop environmentally friendly methods for lithium isotope separation, flowsheets for the recovery and purification of 238Pu to fuel the nation’s space exploration missions and of 63Ni to enable sensitive explosives detection, and separations methods for extracting rare earths for CMI. ORNL’s expertise was used to develop the Next-Generation Caustic Side Solvent Extraction process for the extraction of cesium from alkaline waste that is enabling the cleanup of more than 34 million gallons of high-level tank waste at DOE’s Savannah River Site.

As the national steward of uranium science and processing technology, ORNL uses this core capability to develop chemical separations techniques and measurements that support the validation of modeling and simulation (M&S) tools and enable advances in stable isotope enrichment; used nuclear fuel (UNF) reprocessing; waste treatment technology; production of important radioisotopes (including 252Cf, 238Pu, and 63Ni); radiochemical separation and purification of 249Bk, 251Cf, and other actinide isotopes in support of super heavy element discovery science; and development of isotope applications for NP and other customers. Innovative chemical processes being developed for recovery and recycle of non-nuclear materials from UNF assemblies have great potential for simplifying secure UNF disposition pathways and for reducing the mass and volume of the waste stream. This expertise also enables ORNL to contribute to advances in energy efficiency, renewable energy, fossil energy, waste management and environmental remediation, and national security. For example, physical and chemical techniques for

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carbon capture, with applications for reducing greenhouse gas (GHG) emissions, are being examined using novel adsorbents, including nanostructured materials and ionic liquids.

Chemical engineering research at ORNL makes use of unique resources that span radiological laboratories and nuclear facilities, including the Radiochemical Engineering Development Center (REDC), biochemical laboratories for investigating environmental and biofuels technologies, and chemical and materials laboratories for synthesis and characterization resources. These resources include SNS, HFIR, CNMS, OLCF, and NTRC.

Funding for chemical engineering originates from several sources, including SC [mission areas SC-11, 14, 31], EERE [mission areas ES-1, 3, 5, 8, 11, 15], NE [mission area NE-3], DOE’s Office of Environmental Management (EM) [mission area EM-3], DHS [HS-3], NNSA [mission area NNSA-2], and SPP programs.

7. Chemical and Molecular Science

ORNL's core capability in chemical and molecular science is focused on understanding, predicting, and controlling physical and chemical processes at interfaces over a broad range of length and time scales. This portfolio includes fundamental research programs in catalysis, separations, interfacial analysis (including mass spectrometry and optical spectroscopy), and geochemistry. This program provides fundamental knowledge that serves as a basis for the development of new materials and processes for energy generation, storage, and use; for mitigation of environmental impacts of energy use; and for national security. For example, the Fluid Interface Reactions, Structures and Transport (FIRST) EFRC led by ORNL focuses on developing fundamental understanding and validated predictive models of the nanoscale environment at the fluid–solid interface by taking advantage of neutron and x-ray scattering, spectroscopy, and other characterization tools, coupled with precise synthesis and computational modeling. As part of this EFRC, the surface termination present in layered 2D materials was elucidated by combining neutron total scattering with multilevel structural modeling, which leads to new understanding of structural properties, prediction of chemical and physical properties, and the design of new materials with tailored properties. As part of our chemical imaging studies, novel mass spectrometry, optical spectroscopy, and scanning probe methods have been developed to characterize interfaces and interfacial processes. Many of these advances have been licensed to industry, including femtosecond transient absorption microscopy to spatially and temporally probe the coexistence of free-charge carriers and excitons in heterogeneous photovoltaic materials.

ORNL is computationally designing a new generation of molecular recognition agents with higher selectivity and control in ion separations. This knowledge enabled the selective crystallization of sulfate from complex aqueous solutions via self-assembly, as well as the capture of carbon from gas stream by novel ionic liquids and porous organic polymers. ORNL’s advances in fundamental chemical sciences programs in separations, geoscience, interfacial chemistry, and synthesis science, are being applied to address key challenges for many DOE applied programs. For example, fundamental knowledge from our chemical sciences program is being applied in the EERE-funded CMI, including application of efficient ligands for improving extraction of critical materials.

ORNL is a leader in the use of neutron scattering methods to address fundamental problems in chemical and molecular sciences, such as the structure and dynamics of fluids, solids, and interfaces. For example,

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neutron scattering in combination with reactive transport modeling was used to understand how nanopore processes in caprock of naturally CO2-charged aquifers led to sealing enhancement as a result of coupled geochemical reactions and fluid transport limitations. These strengths also support our activities in catalysis and chemical transformations, where efforts are focused on understanding and controlling reaction selectivity through tuning cooperativity in multi-functional catalysts. Researchers also extensively use CNMS for specialized synthesis and characterization tools, especially world-class electron and scanning probe microscopes (SPMs), and OLCF for computational resources. For example, a unique SPM combined with a density functional theory approach was developed to determine the elastic properties of a 2D battery electrode for the first time which provides new understanding of ionic transport in 2D materials. The chemical and molecular science core capability also comprises novel characterization tools including solution and solid-state nuclear magnetic resonance, surface sampling mass spectrometry, and femtosecond laser spectroscopy.

Funding comes primarily from SC [mission areas SC-7–9, 11, 14]. Applied programs sponsored by EM [mission areas EM-2, 3], NE, EERE [mission areas ES-8, 15] and BER [mission area SC-14] closely couple to the Chemical and Molecular Science core capability.

8. Climate Change Science and Atmospheric Science

ORNL’s core capability in climate change and atmospheric sciences is focused on improving the understanding of causes, impacts, and predictability of climate change by (1) conducting large-scale, long-term, complex ecosystem experiments and observations; (2) leading DOE Earth system model (ESM) performance, workflow, and terrestrial model development (e.g., Accelerated Climate Modeling for Energy); (3) investigating and quantifying climate system feedbacks using ESM simulation experiments constrained by observation and experimental results; (4) integrating multidisciplinary research connecting data, terrestrial, and atmospheric science and large-scale computing; (4) developing novel software to improve credibility and scalability of next-generation climate models in preparation for exascale computing (e.g., International Land Model Benchmarking project, Land-Ice Verification and Validation Toolkit); and (5) utilizing computing expertise and HPC data/infrastructure to improve climate modeling tools.

ORNL advances next-generation integrated models of the human-earth system by improving the characterization of ecosystem processes and land-atmosphere exchange of carbon, nutrients, water, and energy. The Spruce and Peatland Responses Under Climatic and Environmental Change (SPRUCE) and the Next-Generation Ecosystem Experiments (e.g., NGEE–Arctic) projects are large-scale experimental and observational studies conducted in a variety of climate-sensitive ecosystems. ORNL leads in the use of data from these long-term experiments to improve the representation of key plant and microbial traits and their contributions to carbon and other biogeochemical cycles in high-resolution terrestrial biosphere models and ESMs. These sophisticated computer models are increasingly including components of human-dominated systems (e.g., land use, land cover change, and urbanization) and critical interdependencies among energy infrastructure and water resources. ORNL is the premier data resource for the ARM program, which provides key atmospheric radiation measurements from around the world to improve understanding of atmospheric dynamics and cloud processes. ORNL is also the lead institution for the NASA-funded DAAC for biogeochemical dynamics. Capabilities in climate and atmospheric sciences allow ORNL researchers to evaluate the risk of climate change and associated extreme events on terrestrial ecosystems, aquatic ecosystems, and coupled energy and water systems. By incorporating that knowledge into decision support tools, ORNL provides insights into adaptation

strategies and energy security implications. These efforts provide the scientific basis to enable a more resilient and secure US energy infrastructure.

Unique ORNL infrastructure supporting climate change science and atmospheric science activities includes petascale computing (OLCF), which supports M&S and big data applications, state-of-the-art greenhouses, field and laboratory facilities (e.g., SPRUCE), and neutron sources (SNS, HFIR), which enable characterization of soil organic matter and imaging of whole plant/soil systems and plant-water interactions. CADES provides domain scientists with easy access to powerful computing, storage, advanced algorithms, and computational tools.

SC [mission areas SC-3, 13, 16] is the primary sponsor for these efforts; NNSA, NASA, DoD, DHS, the US Geological Survey (USGS), NOAA, and the US Forest Service also sponsor or collaborate on activities that leverage DOE investments in climate change and atmospheric science to generate solutions for the nation.

9. Computational Science

Computational science at ORNL is focused on the development and delivery of scalable computational applications and data analytics [e.g., CASL Virtual Environment for Reactor Applications (VERA), DCA++, QMCPAC, Bellerophon Environment for Analysis of Materials (BEAM)] for current and future leadership computing platforms. These resources enable integrated, scalable solutions of complex problems of interest to DOE and other sponsors, including materials design, nuclear reactor efficiencies and lifetimes, fusion plasma containment, climate change science, health and quantitative biology, and scalable analytics to address complex problems associated with the food-energy-water nexus and global security.

This core capability resides within the world’s most capable complex for computational science, which comprises outstanding staff, infrastructure, and computers dedicated to a research portfolio that covers the full span of ORNL’s interests. ORNL’s expertise in this area is composed of integrated teams of domain scientists, computational scientists, computer scientists, and mathematicians who provide scalable computational and analytical solutions delivered through integration of algorithms, M&S software technologies, computer and information sciences, and HPC infrastructure. These solutions enable transformative science applications that span computational design of new nanomaterials; predictive understanding of microbial, molecular, cellular, and whole-organism systems; simulation of nuclear fission and fusion systems; reliable predictions of climate change at the regional scale, including biogeochemical feedbacks; and supernovae simulation.

The capability also supports early-stage research that addresses problems that are only tractable using HPC for companies of all sizes, including SmartTruck Systems, Ramgen Power Systems, Ford, and Boeing.

This core capability is built upon multidisciplinary teams that tackle science and engineering problems of national interest through the development and application of scalable algorithms requiring tightly coupled workflows that combine experimental data, data analytics, and M&S.

Over the past decade, the ability to efficiently capture, analyze, and steward large volumes of highly diverse data has become increasingly important to ORNL’s sponsors. In addition, data-centric discovery is one of the new frontiers of S&T. ORNL has responded to this situation by creating CADES, an integrated compute infrastructure for delivering data science solutions and workflows that will be sustained and updated over the long term. CADES is effectively creating a new environment for scientific discovery with its diverse computing and data ecosystem, enabling scientists to free themselves from trying to manage, manipulate, and process large data sets.
Funding for this work comes from SC [mission areas SC-1–6, 7–9, 12, 13, 16, 18], NE [mission areas NE-1, 2] and EERE [mission area ES-15]; OE [mission area ES-10], DoD, IC, DHHS, NOAA, and NSF also sponsor or collaborate on activities that leverage DOE investments in computational science.

10. **Condensed Matter Physics and Materials Science**

ORNL has the nation’s largest materials R&D portfolio with world-leading capabilities for predicting, synthesizing, observing, and ultimately controlling materials systems over broad temporal and spatial scales. This makes it possible to ultimately design materials with specific functionalities by connecting the fundamental understanding of complex materials to applications in energy generation, storage, and use. For example, the Energy Deposition Defect Evolution (EDDE) EFRC led by ORNL focuses on elucidating the origin of radiation damage using a unique set of high-entropy alloys combined with atomic-level characterization and computational approaches. The information obtained will be invaluable for designing the next generation of radiation-resistant alloys for nuclear and other applications.

Precise synthesis of materials enables the studies of fundamental properties that ultimately lead to the control of material properties, such as the interactions of 1.8 nm nanoparticles in polymer composites that yielded large effects in polymer properties. ORNL has specialized expertise in synthesis of single crystals, atomically layered oxides, alloys, nanophase materials, polymers, and polymer composites. In addition, ORNL develops unique approaches for characterizing the structure and behavior of materials, making extensive use of key DOE user facilities at ORNL. For example, neutron scattering combined with high-performance computing revealed that ruthenium oxide exhibits a rare combination of antiferromagnetism and metallicity at relatively high temperatures. Further neutron scattering and scanning transmission electron microscopy revealed a new growth mechanism that leads to the formation of highly porous single-crystalline nanobristles. The synthesis and fabrication of complex and precisely controlled nanostructured materials enables new catalytic approaches for CO2 reduction or unique three-dimensional plasmonic nanostructures. To further develop leadership in neutron scattering for basic materials research, ORNL’s experts in materials and neutron scattering have developed a strategic plan to identify key opportunities within the BES-MSE program where neutron scattering will play a critical role. ORNL has also submitted a new proposal, “Understanding Quantum Matter Beyond the Unit Cell,” to examine, using neutron scattering, how topology, spin-orbit coupling, and strong fluctuations intertwine to produce new states of matter. A strategic plan for using neutron scattering to study polymers is presently under development, engaging researchers with many areas of expertise from across the laboratory.

Leadership capabilities in materials imaging, including novel in situ electron microscopy, scanning probe microscopy modalities, atom probe tomography and chemical imaging (such as imaging mass spectrometry and optical imaging), are made available through the user program at CNMS. These imaging capabilities provide direct feedback to materials synthesis, for example via the visualization of

17 D. Lee et al., *Adv. Mater. Interfaces* 4, 160134 (2017)
18 Y. Song, *ChemSelect* 1, 6055 (2016)
individual dopants in two-dimensional materials. ORNL’s experimental condensed matter and materials science efforts are deeply integrated with theory, modeling, and simulation. ORNL has particular strengths in the development and application of scalable computational approaches and codes [e.g., quantum Monte Carlo, Locally Self-Consistent Multiple Scattering] that take advantage of leadership-class computational facilities, including OLCF. ORNL is also developing approaches to apply these codes to next-generation exascale computation as part of a new BES project “Computational Materials Science Center” and another SC Advanced Scientific Computing Research Program (ASCR) Exascale Computing Project.

Activities within this core capability is an important contributor to advances in Applied Materials Science and Engineering (Sect. 3.3) and impacts multiple DOE energy and national security mission areas. This core capability also provided fundamental understanding that helped develop new materials and enhance US competitiveness, as illustrated by many licenses to industry, such as superconducting cables, thin-film batteries, and alumina-forming austenitic steels. In addition, resources developed in this core capability underpin the technologies being developed by CMI.

This work is primarily supported by SC [mission areas SC-7–11]; extensive support is provided through other programs, including FES, EERE, NE, ARPA-E, DoD, the US Nuclear Regulatory Commission (NRC), NASA, and other SPP programs.

11. Cyber and Information Sciences

ORNL conducts cutting-edge R&D in visual analytics, big data analytics, machine and deep learning, knowledge discovery, and information security in order to (1) collect, share, analyze, and classify data; (2) create knowledge from disparate and heterogeneous data sources; and (3) understand, defend against, and defeat known or unknown adversaries to protect the nation’s energy, economic, and security infrastructures. Outcomes from this core capability are translated from R&D to deployment through a partnership with operational cyber infrastructure and collocated expertise in predictive analytics (e.g., social, geographic, visual, graph). ORNL is successfully transferring technologies based on rigorous mathematical results to address cyber and information security challenges, with Hyperion, DataDiode, USB-ARM, Situ, and other tools licensed to multiple parties.

Leveraging our talented scientific staff and unique resources such as OLCF and CADES, ORNL has emerged as a leader in machine learning, information visualization, and heterogeneous data analytics (e.g., graph analytics) at large scale to enable scientific discovery and support the applied programs within DOE and national security agencies. Critical to producing solutions to cyberspace challenges is the ability to acquire, process, and transform massive amounts of data into usable information. ORNL data scientists have a proven track record in developing solutions for customers with diverse data requirements.

ORNL cyber and information security researchers apply strong mathematical rigor and computationally intensive methods, leveraging HPC, to solve cybersecurity challenges at scale and/or in near-real time. Core to the Laboratory’s unique capabilities in this space are statistics, repeatability and reproducibility, observation of trends, and integration of social and behavioral factors, geographic data, and cyber data to yield insights at all levels. ORNL’s unique resources allow for deep learning on HPC systems, which provides unparalleled insights into the behavior of malicious and nefarious cyberspace actors. Quantum information science R&D is providing game-changing capabilities for enforcing cybersecurity on cyberphysical infrastructure systems, such as the electric grid. The unique combination of these capabilities spans areas such as Industrial Control System/Supervisory Control and Data Acquisition (ICS/SCADA) system protection, advanced persistent threat detection and mitigation in networks, and

detection and understanding of malicious code in software and hardware. Furthermore, ORNL develops mathematical methods for identifying the impacts of complex attacks on cyber infrastructures, including software-defined networks, and game-theoretic strategies for ensuring infrastructure resilience in the presence of intentional and incidental disruptions.

Unique ORNL infrastructure supporting this capability includes the Cyber Network Test Laboratory, Distributed Energy Communications and Control Laboratory (DECC), classified HPC systems, Center for Trustworthy Embedded Systems, and Vehicle Security Center. This infrastructure, along with the multidisciplinary staff throughout ORNL in power systems, power electronics, nuclear power systems, and transportation research, enables ORNL to tackle cyber physical security challenges for systems such as the electric grid and smart transportation systems.

Funding for this work comes from SC [mission areas SC-1, 3, 5, 6], OE [mission area ES-10], EERE [mission area ES-16], NNSA, IC, US Department of Transportation (DOT), DHS [mission area HS-4], and DoD.

12. Decision Science and Analysis

ORNL’s decision science and analysis research assists a wide variety of decision makers who grapple with compelling local, regional, national, and global issues. Quantitative and qualitative social, institutional, and behavioral research is conducted on topics as diverse as technology acceptability, market transformation, societal implications of emerging technologies, linkages between science or technology and their intended users, and decision making itself. ORNL’s data-driven methods, models, analyses, and tools create knowledge and insights useful in anticipating, planning for, managing, and understanding responses to and the impacts of numerous events and technologies.

ORNL scientists operating at this nexus of technology and decision analysis have established critical capabilities and expertise in the practice of data-driven decision science, risk analysis, and uncertainty quantification and propagation that are necessary to address impacts of technologies on environmental systems, market dynamics, regulation, and other social factors. These impact assessments are complex, cross-disciplinary, data driven, and often computationally demanding. ORNL’s capabilities and expertise enable the observation, modeling, analysis, and simulation of physical, social, economic, and governance dynamics with unprecedented spatial and temporal resolution, providing an unparalleled opportunity for scenario-driven analyses and evaluation of the consequences of current and future technologies and policies. For example, ORNL uses geographic information science for decision/risk analysis of critical infrastructure expansion (e.g., solar panel adoption). Topical experts integrate patterns and trends in high-dimensional data with physical and human factors, including economics, health, education, and political stability, to glean trends and responses to technological and policy changes on a global scale. ORNL supports DOE and other agencies in strategic planning and program direction, policy formulation, and implementation and is a leader in performing risk analysis of extreme events for siting critical infrastructure.

ORNL is a demonstrated leader in a number of areas within this capability, including (1) spatial demography, geographic data analytics, and techno-social analytics; (2) data-driven decision science, risk analysis, uncertainty quantification, design of experiments, and probabilistic risk assessment; (3) dosimetry and development of dose coefficients and cancer risk factors for human exposure to radionuclides; (4) power plant siting and advanced fuel cycle performance; (5) climate change impacts, adaptation, and vulnerability modeling and assessment; (6) energy economics; and (7) development of decision support tools.

Funding for this work comes from SC [mission areas SC-1, 3, 13], NE [mission area NE-1], EERE [mission area ES-8, 3], DHS [mission area DH-7], the Federal Emergency Management Agency (FEMA), NRC, and the Food and Drug Administration (FDA).
13. Earth Systems Science and Engineering

ORNL researchers analyze the ecological interactions of, and develop quantitative indicators for, the impacts of human activities, natural disturbances, and varying climatic conditions on spatial patterns and processes on the Earth’s surface and near-surface environmental systems. Activities enabled by this core capability include (1) linking a fundamental understanding of mercury biogeochemistry to engineering applications to advance the development of transformational solutions for local legacy mercury contamination; (2) applying highly sensitive tracers in CO2 capture and storage to validate the integrity of CO2 geosequestration; (3) identifying and modeling ecological functions of river and streams within the advanced site selection, design, and operational decision support systems for hydropower and water-dependent thermoelectric technology (e.g., integrating biological and engineering expertise within ORNL’s aquatic research facility to study fish passage mechanics); and (4) developing and assessing sustainability indicators for bioenergy feedstock production and hydropower development through integration of landscape and aquatic ecological science and socioeconomic analyses.

This capability supports DOE’s energy and environmental missions and contributes to the technical basis for policy decisions. ORNL takes advantage of laboratory- to field-scale resources and expertise in geochemistry, hydrology, microbial ecology and genetics, aquatic ecology, and engineering to evaluate the impacts of energy production, transmission, distribution, and use on the environment.

Relevant leadership areas for ORNL include (1) novel integrated sensor and monitoring networks for long-term assessment of environmental change in response to energy production and use; (2) understanding of contaminant cycling and fate in ecosystems to inform the development of innovative remediation technologies and improve risk-based decision-making; (3) assessing impacts of energy production and distribution systems, including existing and advanced hydropower developments, on aquatic ecosystem integrity through sensor systems, novel geospatial analyses, and modeling to identify thresholds and promote adaptability of monitoring and management regimes; (4) modeling and assessing biomass feedstock resources and the logistical and environmental effects of supplying biomass to facilities producing biomass-based fuels, power, heat, or bioproducts; and (5) technologies, systems analysis, and decision support for sustainable hydropower and other energy production and water use.

ORNL’s earth system science and engineering projects take advantage of world-class experimental and computational infrastructure, including neutrons at SNS and HFIR, data infrastructure (CADES), HPC infrastructure (e.g., Titan), state-of-the-art greenhouses, field and laboratory facilities (including the Environmental Science Laboratory, Aquatic Ecology Laboratory, Mercury SFA Field Site, Integrated Field Research Challenge Site, and Advanced Microscopy Laboratory), JIBS, the Center for Bioenergy Sustainability, and CNMS. Funding comes from SC [mission areas SC-13, 14, 15], EM [mission areas EM-1–3], EERE [mission areas ES-3, 8, 9, 10], FE [mission area FE-1], NNSA [mission area NNSA-1], DoD, NE, and NRC.

14. Environmental Subsurface Science

ORNL’s core capability in environmental subsurface science is foundational to advancing the fundamental understanding of processes that control biogeochemical transformation and fate of trace metals in complex, heterogeneous, and multiscale environmental systems. Examples of activities supported by this core capability include (1) delivery of a predictive understanding of complex, heterogeneous, multiscale environmental systems to describe uranium fate and transport in subsurface systems (e.g., through the ENIGMA consortium’s demonstration of “founder” effect and memory response in subsurface microbial communities); (2) field- to molecular-scale geochemistry and microbiology to enable discovery of the genes responsible for mercury methylation and their organismal and environmental distribution (explaining the concentration of methyl mercury in rice and highlighting the potential for massive mercury methylation in the Arctic); (3) state-of-the-art subsurface hydrology
and reactive transport model development; and (4) integration of neutron scattering and HPC to understand enzymatic mechanisms for metal transformation in subsurface systems.

ORNL’s strengths in predicting the state, flux, and residence times of trace metals, nutrients, and contaminants in environmental systems contribute to basic and applied R&D programs focused on extraction of fossil energy, disposal of nuclear waste, and cleanup of legacy contamination. ORNL leads one of the world’s largest ongoing efforts in mercury research. The Critical Interfaces SFA is a multi-institutional, interdisciplinary program that integrates ORNL’s leadership expertise in molecular- to field-scale hydrology, geochemistry, microbial ecology and genetics, biochemistry, and computational modeling to advance a predictive understanding of exchange and feedback processes in low-order streams. The ENIGMA consortium also takes advantage of ORNL’s expertise and field site to improve the understanding of complex, heterogeneous, multiscale environmental systems with an emphasis on the role of subsurface microbial communities in regulating groundwater chemistry.

This core capability comprises a wide range of state-of-the-art facilities at ORNL, including the Critical Interfaces SFA Field Site, the Integrated Field Research Challenge Site, SNS, HFIR, OLCF, CADES, and CNMS. Other DOE user facilities at other national laboratories (e.g., Stanford Linear Accelerator Center, Advanced Photon Source, Environmental Molecular Sciences Laboratory) are also utilized.

Funding comes from SC [mission areas SC-14, 15], EM [mission areas EM-1–3], FE [mission area FE-5], NNSA [mission area NNSA-1], DoD, and NRC.

15. Large Scale User Facilities/Advanced Instrumentation

ORNL has a distinguished record in developing and operating major facilities for DOE and in designing and deploying advanced instrumentation. ORNL is notable for the breadth of the facilities and instrumentation that it develops and deploys for DOE and for its integration of these assets to deliver mission outcomes. The user facilities at ORNL attract thousands of researchers and support the development of the next generation of researchers exploring science and developing technologies that are important to humanity.

SNS and HFIR together provide the world’s foremost neutron-based capabilities for studying the structure and dynamics of materials, biological systems, and basic neutron physics. SNS is the world’s most powerful pulsed spallation neutron source. For neutron scattering experiments that require a steady-state source, HFIR offers thermal and cold neutron beams that are unsurpassed worldwide. Thirty neutron scattering instruments are available to scientists at SNS and HFIR, and the Fundamental Neutron Physics Beamline is available at SNS. Significant investment in instrument improvements, sample environment, and data analysis capabilities make ORNL’s neutron scattering instruments world leading. ORNL has begun conceptual design and preparation of Critical Decision-1 (CD-1) for the Proton Power Upgrade (PPU) and the Second Target Station (STS), a high-brightness short-pulse target station at SNS. The PPU and STS upgrades to SNS leverage DOE’s investment in neutron sciences. PPU will increase the neutron peak brightness and flux at SNS, increasing scientific capacity and capability on currently oversubscribed instruments. PPU also provides the platform for the STS. In addition, HFIR’s capabilities for isotope production, materials irradiation, neutron activation analysis, and neutrino research make it a unique asset for radioisotope, materials and fuels irradiation, and nuclear security sciences.

The HPC resources of OLCF, including the Cray XK7 Titan, are available to users to solve computationally intensive scientific problems and to accelerate innovation for industry partners. ORNL’s other strategic HPC resources include the Cray XC40 Gaea system, operated for NOAA to facilitate multi-agency cooperation and R&D partnerships across the climate research community. Moving forward, ORNL will be fielding Summit, a next-generation, pre-exascale, hybrid platform that will provide 200 PF of computing power for modeling and simulation research, and over 3 exa-ops of computational power for
artificial intelligence (AI) applications and research. Preparations are well underway to facilitate the Summit deployment starting in the end of FY 2017, with production capabilities targeted for the start of calendar year 2018. ORNL is also building the infrastructure required for an experimental computer science facility.

CNMS comprises forefront instrumentation and expertise in nanofabrication, synthesis, and characterization of inorganic nanomaterials and organic polymers and in enhancing the understanding of the structure, dynamics, and functionality of nanostructured materials. Studies of nanoscale structure in soft matter use site-specific deuteration capabilities that enable unique neutron experiments. Development of instrumentation and methods emphasizes new imaging capabilities, with a focus on quantitative measurements of functional properties using scanning probe microscopies, state-of-the-art scanning transmission electron microscopy, atom probe tomography, helium ion microscopy, and chemical imaging. New approaches for direct-write nanofabrication, using electron or ion beams, are also being advanced. Theoretical, computational, and data analytical approaches underpin the research activities across all areas of work at CNMS.

ORNL is home to three major research facilities sponsored by EERE: MDF, which includes the pilot-scale CFTF; the Buildings Technology Research and Integration Center (BTRIC), reinvigorated with the addition of the Maximum Building Energy Efficiency Laboratory (MAXLAB); and NTRC. These facilities enable R&D and demonstration of innovations in renewable electricity generation; energy-efficient homes, buildings, and manufacturing; and sustainable transportation. This cluster of industry-facing facilities enhances engagement with industry and provides a linkage to SC user facilities with complementary capabilities. For example, NTRC researchers have collaborated with industry to use HFIR’s neutron-imaging capability for capturing dynamic images of fuel injectors, and OLCF’s computational resources are being used to provide a better understanding of the materials properties obtained under varying additive-manufacturing conditions and parameters.

Large-scale user facilities and advanced instrumentation are fundamental to ORNL’s ability to deliver on its mission for DOE, DHS, and other customers. Work in this area is supported primarily by SC [mission areas SC-5, 10, 12, 13, 14, 16, 17, 18, 30, 34, 35] and EERE [mission areas ES-5–7], with contributions from NE [mission area NE-1], NNSA [mission area NNSA-1–3], and DoD.

16. Mechanical Design and Engineering

ORNL has extensive experience in the mechanical design and engineering of remote systems and equipment for nuclear applications (e.g., reactors, accelerators, fusion experimental devices, spallation sources, and instruments). This experience includes the seminal development and continued advancement of enrichment technologies manifested today in the development of new stable isotope enrichment systems. Expertise in the analysis of stress, strain, and thermal effects in composite materials and in the dynamic analysis of rapidly rotating devices has been developed in support of these efforts. ORNL has leveraged its access to basic science and scientific tools to innovate solutions for practical mechanical applications. For example, HFIR’s neutron scattering capabilities have been applied to map residual stress in manufactured components to help improve material reliability and to reduce mass in agricultural vehicles, transportation vehicles, and the space shuttle. This capability also has been used to improve additively manufactured components, such as heat exchangers and fuel injectors. Further, ORNL translates research into mechanical design and engineering practice for improvement in energy-efficient manufacturing; in the energy efficiency and durability of building envelopes, equipment, and appliances; and in transportation (multi-cylinder combustion R&D, exhaust after-treatment development).

ORNL has developed remote systems for SNS, REDC, and, most recently, Facility for Rare Isotope Beams (FRIB). Also, ORNL combines its expertise in mechanical design and engineering with other disciplines to
support the Laboratory’s nuclear facilities. This capability is applied to a wide range of challenging problems, including the thermal/hydraulic design of HFIR irradiation experiments, the HFIR closed-loop supercritical-hydrogen cold neutron source, a novel molten salt experimental loop facility, the SNS mercury target systems, and the High-Heat-Flux Diverter components for the Wendelstein 7-X (W7-X) superconducting stellarator. ORNL has designed and fabricated high-speed isotope separation centrifuges for both stable isotope separation and uranium enrichment. This work requires state-of-the-art design expertise with modern materials and precision manufacturing techniques.

ORNL’s interdisciplinary teams of engineers and scientists perform R&D to address the needs of industry, helping to reduce risk and accelerate commercialization of energy-efficient technologies on industry’s timescale. Leveraging ORNL’s leadership in manufacturing innovation into energy-efficient transportation, homes, and buildings enables the achievement of EERE’s manufacturing goals, which aim to increase US competitiveness in the production of clean energy products and to increase US manufacturing competitiveness across the board by increasing energy productivity.

ORNL scientists and engineers are providing the fundamental science for next-generation manufacturing technology that is affecting multiple industry sectors. They are providing knowledge that is accelerating the deployment of new vehicles and efficient transportation systems powered by domestic, renewable, and clean energy. Also, through use of extensive experimental facilities and advanced hardware-based design models, and through incorporation of emerging materials, ORNL’s expertise in buildings technologies has helped industry launch some of the most energy-efficient building equipment technologies on the market today.

ORNL’s applied research facilities (MDF, CTF, BTRIC, NTRC, and the remote systems development high-bay facility) support work by staff with expertise in robotics and remote systems design, thermal hydraulics, energy-efficient manufacturing, transportation, homes, and buildings. Funding in this area originates from several sources, including the SC [mission areas SC-10, 17, 19, 30], NE [mission area NE-1], EERE [mission areas ES-13–15], NNSA, and SPP programs.

17. Nuclear Engineering

ORNL expertise in handling and processing unirradiated and irradiated nuclear materials, developing and operating nuclear reactors, and radiation detection predates the formal discipline of nuclear engineering. In fact, the Oak Ridge School of Reactor Technology, founded at ORNL in 1950, provided the only comprehensive postgraduate nuclear engineering education until the 1960s. This legacy continues as ORNL leads nuclear fuel and irradiated materials S&T; M&S for reactor physics and radiation transport, reactor systems, and reactor safety; radiation detection and imaging; and radioisotope production. ORNL operates world-class nuclear research facilities and leads the US ITER Project Office (USIPO), playing a central role in the nuclear engineering design of the world’s largest fusion experiment.

ORNL’s nuclear engineering expertise is critical to the continued viability of the nuclear power industry, including improved operations and life extension of the existing fleet. ORNL’s expertise in the design and post-irradiation examination of HFIR irradiation capsules is used to study reactor materials and accident-tolerant fuels. ORNL applies modern tools to carry out optical, scanning electron, and transmission electron microscopy as well as chemical, physical, and mechanical property measurements on irradiated fuel and structural materials in support of reactor and UNF systems R&D. ORNL contributes to advanced next-generation reactor technology through the development and testing of new fuels and materials, improved instrumentation and controls, regulatory research, thermal-hydraulic experiments, and innovative system concepts. ORNL is the world leader in molten salt reactor technology, collaborating domestically and internationally to advance the concept’s maturation through M&S, development and operation of liquid salt flow loops for component and material testing, and system studies to ensure
safe and efficient operations. ORNL is also engaging industry on the development of advanced reactor concepts.

Through the development and application of computational analysis tools and nuclear data to advance the scientific understanding of observed phenomena, ORNL is solving complex problems that improve the efficiency and safe utilization of nuclear systems. The ORNL-developed SCALE code is applied worldwide to perform design and safety analysis for reactor and nuclear facilities. ORNL’s hybrid deterministic Monte Carlo methods have transformed computational radiation transport and have enabled reliable, high-fidelity solutions for large-scale, complex problems. ORNL leads CASL, which combines nuclear engineering and HPC to provide a high-fidelity virtual reactor capability that has been validated using operating cycles of the Tennessee Valley Authority’s Watts Bar pressurized water reactors (PWRs). CASL continues to provide scientific understanding to improve the operation of PWRs, boiling water reactors (BWRs), and small modular reactors. In support of ITER, ORNL has developed innovative neutronics modeling tools such as ADVANTG, making it possible to calculate neutron fluxes faster and more accurately.

ORNL’s expertise in uranium enrichment, the nuclear fuel cycle, radiation detection and imaging, and nuclear systems M&S enables nonproliferation and safeguards research that has been vital in supporting negotiations of global nonproliferation agreements. The Nuclear Materials Identification System (NMIS) and the On-line Enrichment Monitor (OLEM) are two examples of ORNL imaging and detection technologies currently having worldwide impact. ORNL nuclear forensics research employs the HFIR neutron activation analysis laboratory, modeling of post-detonation physics, and inverse modeling of reactor depletion and radiation transport. Government agencies depend on ORNL experience in nuclear material processing, handling, and transportation security. For example, ORNL’s Mobile Uranium Facility is positioned to be deployed worldwide to support emergent security missions.

ORNL nuclear engineering efforts employ HFIR; the hot cells of the Irradiated Fuels Examination Laboratory, the Irradiated Materials Examination and Testing Laboratory in Building 3025E, and REDC; other radiological facilities; and OLCF. Funding in this area comes from several sources, including NE [mission areas NE-1–5], SC [mission areas SC-3, 31, 32], NNSA [mission areas NNSA-1–3], DHS [HS-1], the Defense Threat Reduction Agency (DTRA), NASA, NRC, and other government agencies.

18. Nuclear Physics

ORNL’s core capability in nuclear physics spans theoretical and experimental research that is relevant to DOE’s mission of developing an understanding of nuclear matter that will help unlock the secrets of how the universe is put together. Low-energy nuclear experimental research at ORNL focuses on understanding properties of very neutron-rich nuclei through beta-decay spectroscopy, low-energy nuclear reactions relevant to astrophysics, and gamma-ray spectroscopy. ORNL leads aspects of the Separator for Capture Reactions (SECAR) astrophysics detector development and gas jet target development for secondary beams at FRIB. In addition, OLCF is used to investigate the structure and reactions of neutron-rich rare isotopes and nuclear astrophysical processes. For example, calculations indicated that 78Ni is a doubly-magic nucleus with a strong spherical shell closure.21 Such predictions may be tested at FRIB.

ORNL has special expertise in neutron physics, focused on SNS, that includes the development and operation of the Fundamental Neutron Physics Beamline (FnPB). One experiment planned for the FnPB includes the ORNL-led search for the neutron electric dipole moment (nEDM). The nEDM instrument is being designed to improve the sensitivity of detection by a factor of 50 to 100 over previous experiments and to make precision tests of symmetry principles underlying the Standard Model of

particle physics. ORNL leads the development of light-collection devices and low-temperature, high-electric-field electrodes for the experiment, drawing on the Laboratory’s core capability in materials science. For example, ORNL-designed deuterated polymers have been employed in the nEDM electrodes.

ORNL leads research that supports the ton-scale 76Ge Majorana experiment, which will search for the hypothesized neutrinoless double-beta decay mode of nuclei. The Majorana Demonstrator (MJD) project, a feasibility demonstration for the ton-scale Majorana experiment, is currently taking data at the Sanford Underground Research Facility in South Dakota. ORNL expertise in the development of specialized electronics and detectors designed for this project is also relevant to research at Brookhaven National Laboratory and at the Large Hadron Collider (LHC) at CERN, where ORNL researchers conduct relativistic heavy-ion collision experiments to investigate the physical properties of the quark-gluon plasma. ORNL continues to be the lead laboratory for upgrades of LHC’s ALICE heavy-ion detector.

ORNL’s core program in nuclear physics is closely coupled with the NP Isotope Program. A major accomplishment of this program is the discovery of element 119 and new isotopes of element 117 and their decay products. Observations of element 117e have been confirmed at GSI Darmstadt (Germany) using 249Bk produced at ORNL and with the assistance of nuclear physics researchers. Element 117 has been named tennessine in recognition of the contributions of ORNL, UT and Vanderbilt University. With the recent discoveries of elements with atomic numbers $Z = 113, 115,$ and 117 and confirmation by the International Union of Pure and Applied Chemistry, these elements complete the first seven rows of the periodic table, something that has not occurred in the past 200 years. Further, the discovery of element 117 provides strong evidence for the existence of the predicted island of stability.

The nuclear physics core program also provides actinide targets and sources for other NP projects, drawing on unique capabilities at HFIR and REDC, to expand international collaborations in superheavy element research. Preliminary research indicates success in improving the release of fission fragments from high-capacity 252Cf ion sources. The next ion source for the Californium Rare Isotope Breeder Upgrade (CARIBU) project at Argonne National Laboratory will be manufactured by ORNL later in FY 2017. ORNL’s nuclear data program, recognized for its international leadership, includes differential cross-section measurements, development of evaluation methods and data analysis methods, and data processing. These activities provide nuclear data libraries for radiation transport analysis. Further, ORNL leads the ENDF/B Formats Committee which standardizes all nuclear data formatting.

Funding in this area originates from SC [mission areas SC-22, 23, 28–32] and defense programs [mission area NNSA-1 and SPP sponsors].

19. **Nuclear and Radio Chemistry**

ORNL’s radiochemistry and radiochemical engineering expertise, combined with its unique nuclear infrastructure, enables production, processing, purification, and handling of a wide range of isotopes. Stable isotopes and radioisotopes are produced and are provided for use in a variety of important applications, such as scientific research, medical research, and commercial uses.

For scientific applications, research includes super-heavy element discovery, development of specialized sources, isotope dilution mass spectrometry, radioisotope power source development, and cross-section measurements. Radioisotope applications span a broad range, including cancer treatment and commercial uses. ORNL’s nuclear chemistry and enrichment expertise is applied to maintaining and improving our nation’s uranium enrichment capabilities. The Isotope Business Office at ORNL (part of NP’s National Isotope Development Center) maintains and distributes the US inventory of enriched stable and radioisotopes.
HFIR, which provides the world’s highest neutron flux, is used to irradiate target materials for production of various radioisotopes through the NP Isotope Program. The Nuclear Hazard Category 2 hot cells and laboratories at REDC enable the remote production and post-irradiation processing of heavy actinide targets. The HFIR/REDC complex is the nation’s sole producer of 252Cf and high-specific-activity 63Ni, both of which are important in security and industry. Capabilities also exist for recovery of 225Ac, an increasingly important medical isotope, from 229Th. ORNL radiochemists use hot cells and radiological facilities to process and characterize other important radioisotopes, such as 75Se, used in radiography, and medical isotopes 188W, 227Ac, and 212Pb. HFIR and REDC are also being used to produce 238Pu in support of NASA’s planetary science mission. In addition, 249Bk and 256Cf produced at ORNL are used to produce super-heavy elements such as tennessine.

With support from NP, ORNL is establishing new capabilities for producing research quantities of enriched stable isotopes at the Enriched Stable Isotope Pilot Plant (ESIPP) using both electromagnetic and centrifuge technologies. The electromagnetic separation techniques build on expertise in mass spectrometry at ORNL. This capability will ensure a future supply of critical stable isotopes for research and industry. ORNL is also considering the long-term needs for expanded radiochemistry hot cells to support radiopharmaceutical development. As part of the DOE Isotope Program, ORNL maintains inorganic chemistry and materials laboratories to convert the purified isotopes from their stable storage form to user-specified custom forms. These forms frequently are in the shapes of foils, thin films and coatings, plates, and wires.

ORNL’s nuclear and radiochemistry expertise, extensive radioanalytical capabilities (especially advanced mass spectrometry), and neutron activation analysis capability at HFIR, provide world-leading resources for ultra-trace analysis with applications that include environmental analysis, forensics, and security. Expertise in radiochemical separations, analyses, and nuclear material examinations are being applied to the management of nuclear material such as UNF; the detection of materials important to nuclear fuel cycle management and security; the development of safer, more efficient nuclear fuels; and improvements in nuclear waste treatment. As an example, ORNL recently developed an alternate dissolution/extraction concept for nonaqueous tritium pretreatment that has the potential to eliminate the high-acid raffinate waste stream.

Nuclear and radiochemistry research makes use of unique facilities, including HFIR, REDC, hot cells in Building 3025E, laboratories and hot cells in Buildings 4501 and 3047, and other radiological laboratories. Funding in this area comes from several sources, including SC [mission areas SC-8, 11, 31, 32], NE [mission area NE-3], NNSA [mission areas NNSA-1–3], DHS, DoD, NASA, NRC, and other government agencies.

20. Plasma and Fusion Energy Sciences

ORNL’s core capability in plasma and fusion energy sciences, coupled with its demonstrated abilities in large-scale project management, international collaboration and computational simulation, is applied to support the mission of the FES program. ORNL researchers have decades of experience in collaborating nationally [e.g., General Atomics DIII-D, Princeton Plasma Physics Laboratory (PPPL)] and internationally (e.g., Joint European Torus, Experimental Advanced Superconducting Tokamak, Korea Superconducting Tokamak Advanced Research, W7-X) to solve critical experimental and theoretical problems on the road to fusion energy. Using HFIR and ORNL’s nuclear R&D infrastructure, researchers study the effects of neutron irradiation on plasma-facing and structural materials, including tungsten, copper, and their composites. ORNL leads R&D in plasma theory and applies HPC resources to fusion challenges (e.g., the Plasma Surface Interactions project and the Advanced Tokamak Modeling project supported by the SC Scientific Discovery through Advanced Computing program).
ORNL has distinguished expertise in atomic and plasma boundary physics, plasma heating and fueling systems, and fusion materials science. ORNL applies its broad experimental and theoretical expertise in high-temperature plasma science and strong synergies with materials in extreme environments and computational science programs to develop materials and components that can meet the demands of a burning plasma environment and enable fusion facilities to meet their performance objectives. ORNL is DOE’s lead laboratory for pellet fueling systems and is responsible for providing key enabling technologies and components for ITER. Materials scientists at ORNL conduct fundamental experiments to support development of advanced alloys and silicon carbide composites, the results of which have been leveraged to develop a suite of economical high-strength radiation-resistant steels that derive their properties from a fine dispersion of engineered precipitate nanoclusters.

The USIPO, hosted by ORNL, manages the US contributions to the ITER project. As delegated by DOE, ORNL executes US ITER project activities with its partners, PPPL and Savannah River National Laboratory. US ITER fabrication activities and US participation in the overall project will lead to the capability for creating, sustaining, and studying burning plasmas, the next major step toward fusion energy. As the pace of ITER construction has increased, the USIPO has placed substantial procurement contracts with suppliers for component fabrication. US hardware contributions include the central solenoid (the world’s highest-stored-energy pulsed superconducting magnet); a 1 GW cooling water system; high-power, long-pulse plasma heating systems; electrical power components; parts of the tritium exhaust system; plasma instrumentation; plasma disruption mitigation systems; and plasma fueling systems. The USIPO also works with the ITER Organization and other domestic agencies to achieve the required integration of management, design, and procurement activities. The United States was the first to deliver any ITER plant components and the first to deliver an “exceptional heavy load.” Components delivered to date include a set of five nuclear-qualified drain tanks for containing radioactive water from the vacuum vessel and blankets/diverter, the full scope of toroidal field coil conductor (work package completed in February 2017), and major components of the steady-state electrical network (scheduled for completion in FY 2017). Fabrication of the central solenoid is well underway.

Facilities supporting this core capability include HFIR for materials irradiation; hot cells for materials handling and testing; the Irradiated Materials Examination and Testing Laboratory and the LAMDA laboratory for materials characterization; the Fusion Pellet Laboratory for testing and commissioning systems for use on fusion experiments around the world; and the Prototype Materials Plasma Exposure Experiment (Proto-MPEX) for testing the source concept for MPEX, which will provide a world-leading capability for plasma-materials interface studies.

SC funds the work in this area [mission areas SC-17–20], including the US ITER project. Additional funding is received via SPP sponsors.

21. Power Systems and Electrical Engineering

ORNL researchers deliver innovations in power flow, electric grid modernization, energy-efficient buildings and transportation, and smart manufacturing. For example, ORNL has developed high-performance inverters and converters for electric vehicles and demonstrated the first wireless bidirectional charging and energy management system for a building and vehicle operating as an integrated energy system. This core capability (1) delivers advances in high-temperature, high-power-density applications; (2) enables high-efficiency transportation and electrification systems to reduce US reliance on foreign oil; (3) develops technologies for power flow control, grid monitoring (e.g., FNET/GridEye) and grid protection that support development of a secure and reliable 21st century electricity delivery system; and (4) creates advanced building sensors, communications, and controls for power management systems to maximize energy efficiency.
Through DOE’s Grid Modernization Laboratory Consortium (GMLC), ORNL addresses the challenges of integrating conventional and renewable electric generating sources with energy storage and smart buildings while ensuring that the grid is resilient and secure to withstand growing cybersecurity concerns (see Sect. 3.12). ORNL tests controllers in multiple environments, including both simulation and full hardware environments on different scales of power and voltage levels (24 to 480 V) as well as different grid configurations and communications protocols.

ORNL leads in the creation of alternating-current power flow control systems for grid control and increased resiliency. An advanced grid requires new materials for power electronics and energy storage devices. ORNL is a leader in power electronics R&D (Vehicle Technologies Office lead laboratory for power electronics) and is taking advantage of resources at NTRC to develop high-power devices to improve reliability and reduce costs. ORNL is leading the way in innovative wireless charging of electric vehicles. In addition to providing an autonomous, safe, and convenient option for charging electric vehicles, wireless charging when applied to dynamic or quasi-dynamic scenarios can provide virtually unlimited range to electric vehicles and removes “range anxiety” and long charging times because the vehicles can be charged continuously while they are in motion.

ORNL designs, develops, and tests new materials capable of supporting cost-effective and higher performing electricity control devices and systems. ORNL collaborates in developing power electronics from concept to prototype and applies its expertise in advanced materials to develop innovative electronics and sensors.

Enhanced cybersecurity measures are required to prevent malicious attacks on energy infrastructure. ORNL’s Acceleration Project for the Smart Grid is a high-profile activity that will improve the efforts for securing smart grid systems.

Expertise gained in supporting a stable energy infrastructure for ORNL operations has been leveraged to facilitate large science experiments at other sites, such as the LHC and FRIB. Current activities leverage broad expertise in electronics for extreme environments, compact high-voltage power supplies, pulsed power conversion, the Internet of Things (connected sensor and Internet framework), RF, and communications capabilities for intelligent systems support.

ORNL supports DOE’s energy mission by providing resources that can be used to catalyze the timely, material, and efficient transformation of the nation’s energy system. Work in this area is conducted using the NTRC Power Electronics and Electrical Machinery Laboratory, the DECC microgrid, and the Powerline Conductor Accelerated Testing Facility; resources for thin-film deposition (inkjet printing, ultrasonic spray, sputtering, evaporation, low-temperature photonic curing); and tools for characterization of materials, devices, and communications. EERE [mission areas ES-13, 14, 15], OE [mission area ES-10], and DOE’s Office of Energy Policy and Systems Analysis (EPSA) are the primary sponsors. SC also benefits from ORNL expertise in this area [mission area SC-30].

22. Systems Engineering and Integration

ORNL’s core capability in systems engineering and integration takes advantage of the Laboratory’s breadth of capabilities. Optimal solutions to pressing energy challenges are developed by (1) integrating expertise in fundamental science, technology, systems engineering, and project management in multidisciplinary and multi-institutional teams; (2) leveraging large-scale basic and applied science facilities (SNS, HFIR, HPC, OLCF infrastructure, MDF, NTRC, BTRIC, CFTF) to provide foundational science for technology advances (e.g., modeling of combustion processes with industry, understanding materials properties for additive manufacturing, modeling the energy use of buildings at the community scale); and (3) accelerating research innovation in buildings, manufacturing, and transportation through partnerships across ORNL as well as with private industry. ORNL leverages the synergistic potential of collaborations internally across disciplines and externally through multi-institutional collaborations.
ORNL has a successful track record of delivering innovative tools and technologies as a lead and partner on Energy Innovation Hubs (CASL, CMI), the Institute for Advanced Composites Manufacturing Innovation (IACMI), and other multi-institutional collaborations (Fuels/Engine Co-Optima, Grid Modernization Laboratory Consortium, Lightweight Innovations for Tomorrow, Clean Energy Smart Manufacturing Innovation Institute).

ORNL’s strength in pursuing solutions from concept to implementation and in spanning fundamental to applied research ensures the success of national and international science and energy projects such as SNS, Proto-MPEX, ESIPP, ALICE at CERN, ITER, and next-generation fusion experiments. ORNL delivers innovative solutions for manufacturing, transportation, and buildings by applying broad capabilities in materials science and engineering, computational science, decision science and analysis, mechanical design and engineering, nuclear engineering, chemical engineering, and power systems and electrical engineering. This core capability also leverages the development and deployment of large-scale science facilities, systems, equipment, and instruments such as those at SNS, HFIR, REDC, and OLCF.

Additionally, ORNL’s EERE research facilities (NTRC; BTRIC, including MAXLAB and DECC; and MDF, including CFTF) build on ORNL scientific systems infrastructure to develop and deliver market-driven solutions for energy-saving homes, buildings, and manufacturing; sustainable transportation; and power generation. Capabilities and scientific expertise available within these facilities are highly sought after by industry and other sponsors. Recent achievements include combining advanced materials and additive manufacturing to transform wind turbine blade mold manufacturing. Accelerating the fabrication of molds in turn accelerates innovation and reduces the cost of wind turbine development. In addition, ORNL recently manufactured the world’s first 3D printed excavator, which is the first large-scale use of steel in 3D printing.

ORNL’s researchers utilize the EERE facilities as well as SNS, HFIR, HPC, the Vehicle Systems Integration Laboratory, the DECC microgrid, the Ultra-trace Forensic Science Center, the high-bay facility for large-scale components, and remote systems testing. The primary sponsors for these efforts include SC [mission areas SC-10, 17–20, 30–32], EERE [mission areas ES-13–15], OE [mission area ES-10], NE [mission area NE-3], and NNSA [NNSA-2]. Some support is also provided by DHS, NRC, DoD, and other SPP sponsors.

Science Strategy for the Future

Table 4.1. Major ORNL initiatives

<table>
<thead>
<tr>
<th>Initiative</th>
<th>Description</th>
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<tbody>
<tr>
<td>Advance the science and impact of neutrons</td>
<td></td>
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<tr>
<td>Scale computing and data analytics to exascale and beyond for science and energy</td>
<td></td>
</tr>
<tr>
<td>Accelerate the discovery and design of new materials for energy</td>
<td></td>
</tr>
<tr>
<td>Advance the scientific basis for breakthrough nuclear technologies and systems</td>
<td></td>
</tr>
<tr>
<td>Advance the understanding of complexity in biological and environmental systems</td>
<td></td>
</tr>
<tr>
<td>Accelerate research, development, and manufacturing of integrated energy systems</td>
<td></td>
</tr>
<tr>
<td>Deliver science and technology to address complex global security challenges</td>
<td></td>
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</tbody>
</table>

ORNL has established seven major science and technology (S&T) initiatives, listed in Table 4.1, that are strategically aligned with DOE’s mission of ensuring the nation’s security and prosperity by addressing its energy, environmental, and nuclear challenges through transformative S&T solutions. These initiatives are designed to sustain, extend, and utilize the Laboratory’s core capabilities; to provide the scientific and technological focus required to deliver breakthrough solutions in critical national mission areas; and to facilitate the application of these solutions to real-world problems.

In developing these solutions, ORNL will continue to field the interdisciplinary teams that are a hallmark of the Laboratory, partnering with other laboratories, universities, and industry to deliver on its mission objectives, to strengthen our science and innovation culture, and to accelerate the deployment of
As part of this strategy, ORNL has formed four institutes specifically designed to catalyze multidisciplinary R&D. Our science strategy is refined in consultation with the advisory committees established to assess our S&T directorates and with the ORNL Science Advisory Board, which reports to the Laboratory director.

In making Laboratory Directed Research and Development (LDRD) investments, ORNL gives priority to projects that address a set of focus areas that are closely aligned with its major S&T initiatives. Strategic planning at the directorate level informs the LDRD annual call for proposals. In FY 2018, the LDRD focus areas, as outlined in Appendix B, span next-generation data, modeling, and simulation for neutron science; computer science and mathematics for exascale computing and beyond; materials innovation, from atoms to function; nuclear S&T; integrated studies of complex biological and environmental systems; and transformational energy S&T. They also include cross-cutting initiatives in cybersecurity for critical infrastructure, with an emphasis on cybersecurity of the electric grid, and in quantitative biology and genome security. The LDRD focus areas are informed by a set of “Big Science Questions” that could be significant drivers for ORNL research over the next decade. The questions were developed in a cross-Laboratory exercise that involved a diverse group of ORNL R&D staff, including senior, mid-career, and early-career staff.

As part of an ongoing effort to sustain and expand its core capabilities, ORNL has increased its LDRD investment by $2M/year for the past 3 years; in FY 2017, the LDRD budget is $50M (4% of the Laboratory’s operating budget).

**Infrastructure**

**Overview of Site Facilities and Infrastructure**

ORNL, located 10 miles southwest of the city of Oak Ridge, Tennessee, occupies about 4,421 acres of the federal Oak Ridge Reservation (ORR; 34,000 acres). Daily, ORNL hosts ~6,500 people comprising UT-Battelle’s ~4,800 employees, other prime contractors’ staff, subcontractors, and guests. To support its R&D missions, ORNL provides a wide variety of on-site services, including operation and maintenance of all supporting utilities and infrastructure, 24/7 security, dedicated fire and emergency response, medical facilities, unique fabrication and assembly services, a guest house, and other support functions. Work is performed in 209 operational SC buildings (4.6M GSF); in addition, there are 48 operational EM buildings (0.3M GSF). Sixty-nine buildings in shutdown status, owned by SC, EM, and NE, represent 23% (1.5M GSF) of ORNL’s building inventory. This number includes Buildings 3001 and 3019B, which are owned by EM and in shutdown status but not yet excessed.

All SC-mission-unique facilities (1.2M GSF) have an adequate condition rating. Of SC’s non-mission-unique facilities, 91% are rated adequate, with the balance rated substandard except for Building 7012 (which is operating) and various shutdown facilities rated as inadequate. Substandard buildings (which are typically more than 50 years old and underutilized) will be repurposed or excessed. The condition rating for 81% of SC’s operating Other Structures and Facilities (OSFs) is adequate, with the balance (19%) rated substandard. Aged utility systems (i.e., substandard OSFs) are a key focus of modernization.

Research is also conducted in off-site leased facilities (10 facilities totaling 0.23M GSF). ORNL’s Hardin Valley Campus, about 7 miles from the main campus, hosts MDF and NTRC. CFTF is in Oak Ridge, 5 miles from the main campus. Offsite facilities provide ready access for industrial partners. ORNL’s leased space portfolio is evaluated frequently for consolidation and/or reduction opportunities; two leases were terminated in 2016.

ORNL’s Site Wide Master Plan can be found at [https://services.ornl.gov/ronweb/Media/ORNLswmp.pdf](https://services.ornl.gov/ronweb/Media/ORNLswmp.pdf).
ORR land use is governed by the current ORR Land Use Plan (Oak Ridge Reservation Planning: Integrating Multiple Land Use Needs. FY2012 Update. DOE/ORO/2411. Oak Ridge National Laboratory, Oak Ridge, Tennessee).

Campus Strategy

ORNL’s campus strategy is focused on achieving and advancing distinctive scientific missions. The execution of this strategy relies on achieving four primary objectives:

1. Advance science and energy leadership by
   - sustaining world leadership in neutron sciences
   - sustaining world leadership in high-performance computing
   - delivering innovation in materials and manufacturing
   - strengthening nuclear capabilities
2. Establish a modern adaptable infrastructure to support research
3. Return the ORNL central campus to productive science missions
4. Reduce excess facility liabilities

These goals are accomplished through addition of capacity as needed to support research, sustainment and recapitalization of key assets, and deactivation and demolition of excess assets. The most important needs for each objective are identified and addressed through ORNL’s annual Mission Readiness process which culminates in planned facilities and infrastructure investments as shown in Fig. 6.1.

Objective 1: Advance Science and Energy Leadership

ORNL integrates and applies 23 core capabilities (see Sect. 3) to address a wide range of R&D mission challenges. Our campus strategy focuses on four areas of infrastructure investment to advance ORNL’s science and energy leadership and enable accomplishment of the major initiatives described in Sect. 4.

Sustain world leadership in neutron sciences: Continuing to operate SNS and HFIR as world-leading neutron scattering user facilities requires programmatic and infrastructure investments. The proposed PPU at SNS will increase power delivered to the first target station to 2 MW, increase neutron flux on available beam lines, and provide a platform for eventual construction of the second target station (STS). Addition of a STS to SNS, requiring a major programmatic investment, will provide ORNL with three complementary neutron sources and ensure US leadership in neutron sciences for the foreseeable future. At HFIR, depletion of the reactor’s fuel inventory presents a critical mission risk for neutron sciences as well as nuclear S&T programs and isotope production. Additional programmatic funding provided in FY 2016 allowed the Laboratory to keep the HFIR fuel inventory stable, although at a historically low level, while still operating HFIR for an additional cycle. The reactor has been operating at greater than 97% reliability over the past 5 years. However, 41 items threaten reliable operations with respect to plant health. Appropriate investments in plant health will be needed to sustain seven cycle per year operations reliably.

Growth in the use of ORNL’s neutron scattering facilities will create increasing demands on research support functions and thus will require additional infrastructure investments. An experiment support facility at SNS and a sample environment facility at HFIR are needs being discussed with DOE-BES.

Sustain world leadership in high-performance computing: Leadership-class computing underpins almost all key DOE and ORNL scientific disciplines, and continuing evolution of ORNL’s HPC infrastructure is a priority. ORNL’s well-defined path to maintain leadership in HPC includes the installation and operation of the pre-exascale Summit machine (OLCF-4) in 2017–2018 and the deployment and operation of an initial exascale system (OLCF-5) in the early 2020s. ORNL will continue to combine institutional, third-party, and DOE investments to create a highly capable HPC ecosystem, thus providing the backbone for
the programmatic investments needed to field the next two generations of HPC capabilities. To prepare for the acquisition and deployment of the generation of HPC machines following Summit, ORNL has considered various options. A preferred option involves the reconfiguration of the facilities housing the current HPC machines. That option leverages significant prior investments in power and cooling water systems (about $100M) but requires relocating research activities not related to HPC. To facilitate the relocation of non-HPC research programs under the preferred option, and to accelerate the closure of Buildings 4500S and 3500, which will eliminate deferred maintenance of $22M, the construction of the Translational Research Building (TRB) on ORNL’s central campus would be required. A second option to accommodate next-generation computing would be the construction of a new, stand-alone facility also capable of handling “beyond Moore’s Law” research. A facility with some of these characteristics, proposed in 2010 as an alternatively financed project, was not supported by the Office of Management and Budget. ORNL has developed sufficient information to support a CD-0 decision package in the near term for either of the options under consideration.

Deliver innovation in materials and manufacturing: Accelerating the design, discovery, and deployment of new materials and manufacturing processes requires specialized instrumentation and facilities. ORNL has made discretionary investments to secure new world-class tools for materials science including a secondary ion time-of-flight mass spectrometer, a monochromated aberration-corrected scanning electron microscope and a low-temperature 4-probe scanning tunneling microscope. Institutional General Plant Project (IGPP) funds have been allocated and design is under way to provide a facility with low vibration/electromagnetic fields to support increasingly sensitive imaging equipment. IGPP-funded upgrades to Building 4508 are under way to support investigations of materials under extreme environments. MDF provides ORNL and our industry partners with tools for translating scientific discoveries into solutions to revitalize US manufacturing, with a focus on additive manufacturing and production of low-cost carbon fiber and composites. ORNL’s carbon fiber and composites research and unique processing capabilities are critical assets for IACMI. ORNL is exploring additional leased space in the Hardin Valley campus area to support these activities.

Strengthen nuclear capabilities: ORNL’s unique nuclear capabilities are a vital resource for several DOE and other agency programs, enabling the delivery of

- isotope R&D, isotope production, and heavy element R&D for NP;
- fusion and fission materials research for FES and NE;
- nuclear fuel cycle research, strategies for UNF disposition, validation of nuclear systems M&S, and advanced reactor concepts development for NE;
- advances in nonproliferation, nuclear forensics, low-enriched uranium fuels, and domestic uranium enrichment for NNSA; and
- space power and portable power sources for NASA.

These capabilities are critically dependent on three key functions: (1) operation of HFIR as a high-flux irradiation source, (2) processing and handling of irradiated and nuclear materials, and (3) management of radioactive waste. Challenges for HFIR include sustained programmatic support for operations, new fuel fabrication, and spent fuel shipments. Sufficient funding needs to be provided each year to implement planned life extension projects.

Four ORNL buildings (7920, 7930, 3025E, and 3525) currently provide radiochemical processing and irradiated nuclear material R&D capabilities. Efforts are under way to stand-up operations in Building 3047 for medical isotope production and to address the pressing need to update key radiological facilities such as Buildings 4501 and 4505 to accommodate increasing demand for isotope fuel research. Base operating cost (regardless of program workload) for these facilities is $30M/year. Programs provide an additional $8M–$10M annually for the performance of specific work in these facilities. In FY 2016, the base operating cost for these hot cell facilities was covered by shared funding of $18M from
NE and $12M from SC. ORNL will continue to work with SC and NE to ensure that a sustainable financial model supports these assets.

For more than 20 years, SC programs have relied on radioactive waste management systems provided and funded by EM. As EM completes its cleanup of legacy waste in Oak Ridge, many of these aging systems are scheduled for shutdown. Thus, ORNL must deploy sustainable waste treatment system alternatives to manage newly generated transuranic (TRU) solid debris, radioactive liquid wastes (remote-handled and contact-handled TRU and low-level wastes), and gaseous exhaust streams. To mitigate this infrastructure capability gap, institutional investments will be required. Ongoing efforts to address this need include (1) an independent technical review to evaluate alternatives for processing the radioactive liquid wastes and (2) evaluation of liquid waste minimization techniques in chemical
processing activities. ORNL will use findings from these studies to pursue the most cost-effective alternative to manage newly generated wastes, supporting science into the future.

Other institutional investments include a high-bay space for domestic uranium enrichment development; consolidation of stable isotope R&D and production; upgrades to high-bay robotic R&D capabilities; and upgrades to key radiological facilities (e.g., Buildings 4501 and 4505). Additionally, ANML is being proposed to NE to provide world-class materials research, development, analysis, testing, and qualification to underpin fundamental science needs in support of advanced materials for nuclear energy systems.

**Objective 2: Establish a Modern, Adaptable Infrastructure to Support Research**

Over the past 15 years, the research infrastructure at ORNL has undergone substantial improvement. Major scientific user facilities such as SNS and CNMS now serve large user communities. At OLCF, researchers use world-leading supercomputers to accelerate scientific discovery. Other new facilities, including the Chemical and Materials Sciences Building, new greenhouses, CFTF, and MDF, are enabling ORNL scientists to tackle challenging problems in support of the needs of DOE and other sponsors.

During this period of intensive investment in R&D capabilities, resource limitations allowed for only modest institutional investments in the support infrastructure that enables ORNL’s broad portfolio of work. Although the investments have addressed some key needs, significant infrastructure capability gaps remain. For example, investments of ~$12M in the 7000 Area at the east end of ORNL’s main campus have enabled demolition of three obsolete facilities (Buildings 7005, 7018, and 7040); construction of two new facilities (Buildings 7120 and 7122); and improvements in utilities (medium-voltage 13.8 kV foundations and fiber network reconfiguration) and in roads and grounds. Even with these investments, this area remains in need of substantial modernization. To improve support for ORNL’s research facilities, a modernization of the 7000 Area is proposed with support from multiple funding sources.

Capabilities for precision machining and intricate custom metal fabrication capability are vital to ORNL’s research programs and are particularly important for several science missions: (1) SNS and fusion/ITER (high-vacuum work), (2) HFIR (reactor assemblies and components), and (3) several nuclear technology and national security missions. The Laboratory’s existing fabrication facility is more than 60 years old and does not provide the humidity control, temperature control, or clean and reliable electrical power required by modern machine technology. To eliminate this gap, ORNL is requesting an SLI-GPP investment in FY 2018 to renovate the fabrication facility, thereby creating an environment suitable for technologically advanced machining (see Table 6.1).

In the area of emergency response, ORNL is proposing the construction of the Research Operations Support Center (ROSC) as an SLI line item project. The ORNL protective force headquarters and fire station are more than 60 years old with significant deferred maintenance (DM). ORNL’s existing fire station and emergency operations center could not survive a natural disaster, as required for compliance with DOE Standard 1020-2012, and the fire station is not located close enough to SNS and CNMS to consistently meet DOE-required response times. The ROSC will provide compliant, mission-ready facilities to better ensure delivery of emergency and protective force functions that are aligned with the current and planned configuration of the Laboratory’s research facilities (Table 6.2). The facility could be constructed using IGPP resources if the limit on IGPP were raised to $20M.

Demolition of Buildings 7001 and 7002 is crucial to the modernization of the 7000 Area, which houses most of the support services (e.g., fabrication, vehicle services, shipping and receiving) for the Laboratory. These services have, in large measure, been provided from the same facilities since the 1960s. ORNL will use institutional funds for the demolition of Building 7001 in FY 2017. ORNL also plans to invest institutional resources to replace the garage facility (Building 7002). The proposed ROSC and
The renovation of the Materials Fabrication Facility will eliminate gaps in infrastructure capability while reducing ORNL’s DM backlog by $4.6M. Construction of the ROSC will allow for the demolition of Buildings 2500, 3037, 7031, and 7058, eliminating approximately 21,000 ft² of suboptimal space.

Table 6.1. Modernizing ORNL’s machining and fabrication capabilities for 21st century science

| Deliver cutting-edge machining and fabrication core functions | • Precision material machining to <0.005 in.  
• Pedigreed material fabrication  
• Intricate custom metal fabrication |
| Meet modern machining technology requirements | • Humidity-and temperature-controlled environments for precision measurements and machining tolerances  
– Coordinate measuring machine  
– Multi-axis lathes, mills, and live tooling  
• Clean and reliable power |
| Add new capabilities to meet identified needs | • Laser punch machine  
• Jig bore grinder |

Table 6.2. Providing ORNL with a compliant, mission-ready Research Operations Support Center

| Provide modern, code-compliant facilities to support the conduct of forefront science | • Replace obsolete fire station (Building 2500) and protective forces headquarters (Building 3037)  
– Unable to survive a natural disaster, as required by DOE Standard 1020-2012, Natural Phenomena Hazards Analysis and Design Criteria for DOE Facilities  
– Storage of responder personnel protection apparatus in substandard environment  
– Other code and standard deficiencies |
| Consolidate emergency response, emergency management, and protective force functions near ORNL’s geographic center | • Improve efficiency through colocation of functions that are now dispersed in obsolete buildings across ORNL  
• Enable compliance with required response times, increasing the level of protection afforded to personnel and facilities |

Significant resources have been allocated to sustain critical utilities; however, continued aging of utility systems requires additional investments to prevent service disruption. An interruption of key utilities such as sewage treatment, fiber network service, or potable water would have an adverse effect on activities at ORNL. A 10-year investment plan has been developed to restore all critical utility systems to adequate condition.

Objective 3: Return the ORNL Central Campus to Productive Science Missions

ORNL’s East and West campuses have undergone dramatic transformation over the last 15 years, enhancing the Laboratory’s ability to execute key DOE missions and attracting top scientific talent to the Laboratory. However, the Laboratory’s central campus remains largely un-modernized; consequently, liabilities and risk continue to grow. This area is occupied by operational facilities such as the Irradiated Fuels Examination Laboratory (Building 3525), a number of excess facilities slated for decontamination and demolition (D&D); and Building 3019, which houses EM-sponsored 233U disposition operations. ORNL’s security posture and associated costs are driven upward by the continuing presence of the 233U inventory, complicating the Laboratory’s ability to achieve a more open campus for the science mission and impeding central campus modernization. ORNL has proposed several alternatives to accelerating the disposition of the 233U inventory because of the risk that this inventory creates and its significant effect impact on the cost of doing business at ORNL and on its overall security posture.
Execution of the Exascale Computing Project requires the relocation of non-HPC research equipment and staff from Building 5800 (see Sect. 4.2). ORNL’s preferred option is to relocate the research operations to the Translational Research Building (TRB), a new facility whose construction would provide much-needed high-bay space and would eliminate $22M in DM by vacating Buildings 4500S and 3500. It would also serve to advance the modernization of the ORNL central campus.

The Manhattan Project National Historic Park, established in November 2015, includes the Graphite Reactor, a frequently visited historic site on ORNL’s central campus. ORNL is supporting DOE and the National Park Service in their cooperative efforts to manage the park, including improvements to the Graphite Reactor to support an expected increase in visitors.

**Objective 4: Reduce Excess Facility Liabilities**

ORNL expends approximately $3.2M annually on excess facilities to minimize environmental and safety risks. However, these costs are expected to grow significantly in the near term if these facilities are not demolished soon. Some of these facilities also represent barriers to continued modernization of the campus.

Working with DOE’s Excess Facilities Working Group, ORNL prioritized excess facilities into four groups:

- SC and NE facilities at located at the Y-12 National Security Complex (Y-12), including the former Biology Complex;
- 7000 Area facilities;
- high-risk process-contaminated facilities in ORNL’s central campus; and
- balance of buildings for demolition.

The facilities at Y-12 represent the largest cost risk to ORNL due to their deteriorated condition and size. Although the structures in the 7000 Area are not high-consequence facilities, their demolition remains a priority to facilitate the continued modernization of the ORNL main campus. The process-contaminated facilities on the central campus pose an overall risk to the SC missions because they contain a combined radiological inventory of several thousand curies, and significant effort is required to maintain them in a safe and secure configuration.

The waste management systems owned and operated by EM also represent risk to ORNL and SC. These aging, highly radioactive systems for liquid and gaseous waste collection and treatment are located on ORNL’s main campus and include underground transfer lines, ducting, exhaust fans/stacks, and evaporator systems that should be removed immediately upon cessation of operations by EM to prevent negative impacts to ORNL’s mission. If these systems are not addressed in a timely manner, they will create radioactive source terms that present unnecessary risks to the ORNL staff, environment, and mission; necessitating considerable surveillance and maintenance (S&M) investments and impeding modernization. It is critical that SC engage EM in the development of the next ORR EM cleanup contract to ensure that the correct scope is addressed from an SC perspective.

With the closure of Holifield Radioactive Ion Beam Facility as a user facility in 2012, NP is funding partial decommissioning through FY 2017. NP will provide S&M funding for portions of Building 6000 from FY 2018 until the facility is ready for shutdown.

**Future Infrastructure Gaps within a 10-year Window**

ORNL will celebrate 75 years of operation in 2018 and, as discussed in Sect. 6.2, has experienced dramatic renovation over the last 15 years. However, even with significant infrastructure investments, further investments are required over the next decade to recapitalize and sustain aging assets. Utility system improvement priorities include establishment of an alternate source of potable water,
replacement of an aging chiller plant (achieved through chilled water system interconnections) and upgrade of the sewage treatment plant.

A new facility is needed to provide modern office environments for those utilizing the Melton Valley campus. Nearly 100 staff and visiting scientists are currently housed in old, dilapidated trailers scattered through the complex.

Institutional investments are also planned to modernize Buildings 4501 and 4505. These Cold War-era radiological assets support important research in national security and nuclear energy applications, as well as isotope production and development in support of US industries and vital medical research. Renovation of Building 6010 is required to house the stable isotopes program and the National Stable Isotope Repository.

IGPP-funded construction of a multi-program facility is being considered for the 7600 Campus to support the full-scale Materials Plasma Exposure Experiment, the Light Water Reactor Sustainability Program, solid-state battery R&D, and the ITER Pellet System Integrated Testing Laboratory.

Materials with long and reliable service life in extreme environments (e.g., temperature, pressure, chemical, radiation, plasma) are necessary to meet current and future energy systems demands. To meet this need, materials must be economically developed, produced, fabricated and deployed economically, and must be “born qualified” to meet existing and new standards. This goal will be realized by efficiently combining many elements: a fundamental understanding of materials, integrated computational materials engineering, advanced manufacturing techniques, M&S of properties and predicted behavior, and analytical methods. ORNL proposes the construction of ANML to meet this challenge. ANML is envisioned to be a radiological facility providing world-class capabilities for research, development, analysis, testing, and qualification of materials to surpass current performance limits and to extend service life in extreme environments. By combining these capabilities, ANML will deliver a two-fold mission: (1) basic understanding of material behavior in nuclear energy applications and (2) new qualified materials for deployment.

**Infrastructure Investment Summary**

ORNL’s funding priorities in each of the major funding categories are listed in Table 6.3.

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Non-mission-unique facility investments are summarized in Appendix E. Institutional capital and expense investments are the predominant funding sources for continued site modernization. Funding priorities for disposing of excess facilities are identified in Sect. 6.2 and in Appendix E. Maintenance and repair investment is between 2% and 4% of the replacement plant value. Thirty-four percent of ORNL’s operational non-mission-unique facilities, representing approximately 45% of the total GSF, are more than 50 years old and carry nearly 90% of the DM. As shown in Appendix E, DM is expected to remain essentially unchanged until FY 2023, when a significant drop will occur. This drop reflects ORNL’s plan to
reduce DM by deactivating and excessing aging facilities, leading to footprint reduction, and by repurposing older facilities to support current and future mission needs.
PACIFIC NORTHWEST NATIONAL LABORATORY

Lab-at-a-Glance

Location: Richland, WA
Type: Multi-program Laboratory
Contractor: Battelle Memorial Institute
Site Office: Pacific Northwest Site Office
Website: www.pnnl.gov

Physical Assets:
- 582 acres and 77 buildings (DOE & Battelle Facilities)
- 874k GSF in buildings
- Replacement Plant Value: $772M
- 962k GSF in 27 Leased Facilities (Not including Battelle)

Human Capital:
- 4,183 Full Time Equivalent Employees (FTEs)
- 55 Joint Faculty
- 259 Postdoctoral Researchers
- 433 Graduate Students
- 469 Undergraduate Students
- 1,814 Facility Users
- 100 Visiting Scientists

Mission Overview

Pacific Northwest National Laboratory (PNNL), as the nation’s premier chemistry, earth science, and data analytics laboratory, conducts world-leading research and development to address our most challenging problems in energy resiliency and national security. Located in Richland, Washington, PNNL is one of 10 United States (U.S.) Department of Energy (DOE) Office of Science (SC) national laboratories. Operated by Battelle Memorial Institute, PNNL had 4,485 staff and total funding of $1B during fiscal year (FY) 2016.

PNNL has world-leading capabilities in chemical catalysis, data analytics, and integrated earth system sciences. Building upon its strong base of discovery science, PNNL is a leader in energy storage and grid performance and is transforming the way the country operates and maintains its electricity and energy delivery systems. PNNL has developed advanced computing tools that analyze grid congestion faster and more accurately, saving utilities millions of dollars. In national security, PNNL possesses world-leading expertise in forensic signatures of plutonium production, large-scale data analytics, and cyber defense of high-consequence systems. The Laboratory provides critical capabilities to the United States and its international partners to verify international treaties and implement security technologies around the globe.
On behalf of SC’s Office of Biological and Environmental Research (BER), PNNL operates the Environmental Molecular Sciences Laboratory (EMSL) and provides technical and operational leadership to the Atmospheric Radiation Measurement (ARM) Climate Research Facility. The Radiochemical Processing Laboratory (RPL), a Hazard Category II non-reactor nuclear facility, enables innovative radiological material processes and solutions for environmental, nuclear energy, and national security research. PNNL operates DOE’s only facility for marine sciences in Sequim, Washington, building upon a rich history of research related to marine and coastal resources, environmental chemistry, water resources modeling, ecotoxicology, biotechnology, and national security. PNNL also has satellite offices in Seattle, Washington; Portland, Oregon; and College Park, Maryland.

Core Capabilities

PNNL has 19 core capabilities, each a powerful combination of world-class staff, state-of-the-art equipment, and mission-ready facilities. These capabilities represent a collective set of skills and a body of world-leading scientific and engineering work that provides exceptional value and mission delivery to DOE, the National Nuclear Security Administration (NNSA), the U.S. Department of Homeland Security (DHS), and the missions of other federal agencies and industry through our strategic partnership projects (SPPs).

A hallmark of PNNL is our focus on bringing multiple capabilities to bear on complex scientific and technological (S&T) challenges. Synergies among these core capabilities enable PNNL to tackle the fundamental scientific discovery challenges posed by DOE and to deliver transformational research required to accelerate the delivery of solutions to the marketplace. This approach is discussed in the capability descriptions below.

Figure 1 - PNNL has 19 core capabilities grouped into five areas: chemical and materials sciences, computational and mathematical sciences, earth and biological sciences, engineering, and large-scale user facilities and advanced instrumentation.
The 19 core capabilities have been grouped into five (5) areas (see Figure 1):

- **Chemical and Material Sciences** includes core capabilities in: 1) chemical and molecular science; 2) condensed matter physics and materials science; 3) applied materials science and engineering; and 4) nuclear and radiochemistry.
- **Computational and Mathematical Sciences** includes core capabilities in: 5) advanced computer science, visualization, and data; 6) computational science; 7) applied mathematics; 8) cyber and information science; and 9) decision science and analysis.
- **Earth and Biological Sciences** includes core capabilities in: 10) climate change and atmospheric science; 11) earth systems science and engineering; 12) environmental subsurface science; and 13) biological systems sciences.
- **Engineering** includes core capabilities in: 14) nuclear engineering; 15) chemical engineering; 16) systems engineering and integration; 17) power systems and electrical engineering; and 18) biological and bioprocess engineering.
- **User Facilities and Advanced Instrumentation**, includes EMSL and ARM, which represents PNNL’s nineteenth core capability.

PNNL has many core capabilities in which our staff are internationally recognized, including advanced computer science, visualization, and data; applied materials science and engineering; chemical and molecular sciences; climate change science and atmospheric science; cyber and information sciences; decision science and analysis; earth systems science and engineering; environmental subsurface science; nuclear and radiochemistry; nuclear engineering; power systems and electrical engineering; and systems engineering and integration. Most of the remaining core capabilities are nationally recognized and one is an emerging capability (i.e., condensed matter physics and materials science).

### Chemical and Material Sciences

#### 1. Chemical and Molecular Sciences

Chemical and molecular sciences is a core capability that advances the understanding, prediction, and control of chemical and physical processes in complex, multi-phase environments. PNNL has significant domain expertise in condensed phase and interfacial molecular science, chemical physics, catalysis science, chemical separations and analysis, geochemistry, computational chemistry, and actinide science. This core capability has strong ties to the condensed matter physics and materials science, computational science, and the applied mathematics core capabilities, leveraging expertise in those areas to advance our understanding of complex phenomena at molecular liquid-solid interfaces and produce high-fidelity simulations of molecular processes controlling macroscopic phenomena.

The Laboratory has the largest fundamental research effort within the national laboratory system in catalysis science and condensed phase and interfacial molecular science, which provided the foundation for establishing the Institute for Integrated Catalysis. These capabilities were essential for the award and renewal of an Energy Frontier Research Center (EFRC) in Molecular Electrocatalysis from DOE’s Basic Energy Sciences (BES) program and an award from SC’s Early Career Research Program for the project “Combined Capture and Conversion of CO2,” selected by BES. Contributing to PNNL’s strength in this area is EMSL’s computational chemistry software application (NWChem), which is used worldwide to efficiently solve large molecular science problems on computing resources ranging from high-performance parallel supercomputers to workstation clusters. Capability stewardship efforts, such as those proposed in the Energy Sciences Capability (ESC) project, will accelerate scientific discovery in chemical transformations by enabling close integration of synthesis with dynamic characterization capabilities and real-time computation capabilities (for more information on the ESC, see section 6.2, pages 32 and 33 of this plan).
The capability forms the basis for PNNL’s fundamental science programs in catalysis science, condensed phase and interfacial molecular science, computational and theoretical chemistry, geosciences, and separations and analysis. Applied programs include improved energy technologies, catalysis and reaction engineering, hydrogen storage, biomass conversions, environmental remediation, and carbon capture/sequestration. This capability receives support from programs in BES, BER, DHS, DOE’s Office of Energy Efficiency and Renewable Energy (EERE) (geothermal, biomass, and hydrogen; fuel cells; and infrastructure technology), Office of Fossil Energy (FE) (carbon- and co sequestration), the Office of Environmental Management (EM) (environmental remediation), NNSA (nonproliferation), Department of Health and Human Services (DHHS), and the U.S. Department of Defense (DoD). BER’s support of EMSL capabilities also greatly enhances this core capability through the continued focus on molecular transformations that occur in batteries and catalytic systems (including biocatalysts), as well as at complex interfaces. Staff who support the work in these programs are located in the Physical Sciences Laboratory, EMSL, and the Math Building.

2. Condensed Matter Physics and Materials Science

PNNL is an emerging leader in condensed matter physics and materials science, a core capability that provides the knowledge base for discovery and design of new materials with novel structures, functions, and properties. This knowledge serves as a basis for development of new materials for energy generation, storage, and use as well as mitigating its environmental impact. The Laboratory has domain expertise in synthesis of nanostructured and biomolecular materials, in situ electron and scanning probe microscopy, radiation effects and degradation in materials, and computational materials science. This core capability has strong ties to the chemical and molecular sciences, applied materials science and engineering, computational science, and applied mathematics core capabilities. In combination, these capabilities advance our ability to understand and manipulate complex phenomena at solution-solid and solid-solid interfaces, design and synthesize hierarchical matter, and develop computational tools that elucidate the mesoscale principles linking atomistic details of structure and interactions to outcomes of synthesis and function. Capability stewardship efforts enabled by the ESC project will strengthen the strategic link with our world-class efforts in the predictive design and understanding of chemical transformation processes. The ESC project will provide close integration with the chemical and molecular sciences capabilities through emphasis on predictive synthesis of hierarchical materials, enabling a strategic link to this core capability through the need to translate an understanding of catalytic processes into multifunctional catalytic materials.

PNNL has a distinctive strength in the emerging science of materials synthesis, to which it brings synthesis of hierarchical materials, both inorganic and organic; the most advanced imaging and spectroscopy tools, many of which are applied in situ and operando; and computational approaches that draw on PNNL’s long-standing leadership in computational chemical physics, as well as new capabilities in condensed matter theory and computation. PNNL’s capability is particularly strong in understanding the complexity at interfaces, specifically their role in synthesis and their control of the transport of matter and energy. These strengths have advanced PNNL’s research at the Joint Center for Energy Storage Research (JCESR), an Energy Innovation Hub led by Argonne National Laboratory.

This capability forms the basis for PNNL’s sponsor-funded, fundamental science programs in synthesis and processing, biomolecular materials, electron and scanning probe microscopy, mechanical behavior, and radiation effects. Applied programs to which this core capability contributes include radiation effects in materials, multiscale behavior of structural materials, design and scalable synthesis of materials and chemicals that bridge the mesoscale fuel cells and energy storage, electric and lightweight vehicle technology, nuclear reactor safety assessment, regulatory criteria and life extension, and legacy waste forms. This capability receives support from programs in BES, BER, DOE’s Offices of Electricity Delivery and Energy Reliability (OE), the Office of Nuclear Energy (NE), EERE, and National Institutes of Health (NIH). BER’s support of EMSL capabilities (e.g., Quiet Wing and the High Resolution and Mass
3. Applied Materials Science and Engineering

PNNL’s capability in applied materials science and engineering has a strong emphasis on materials synthesis, manufacturing, and device fabrication and testing that can be scaled up and transferred to industry. PNNL has made significant contributions to the commercialization of automobile catalysts, organic light-emitting devices, biofuels, redox flow batteries, and many other clean energy technologies. PNNL has domain expertise in materials characterization; materials theory, simulation, design, nucleation, and synthesis; materials structural and chemical modification; the role of defects in controlling material properties; and materials performance in hostile environments, including the effects of radiation and corrosion. This capability is supported by the Laboratory’s other capabilities in chemical, molecular, biological, nuclear, and subsurface science, as well as the ability to engineer enabling nanostructured and self-assembled materials, tailored thin films, ceramics, glasses, alloys, composites, and biomolecular materials. PNNL is developing advanced glass formulations, key process control models, and tactical processing strategies to ensure safe and successful operations for the high-level and low-level waste vitrification facilities.

The Laboratory leverages this core capability to conduct work in the areas of energy storage materials, solid oxide fuel cells, solid-state lighting, absorption cooling, lightweight alloys, magnetic materials, organic electronic materials, and radiation effects on materials, as well as the synthesis and processing of bulk nanostructured materials, high-surface-area materials, catalysts, and nanoporous materials for energy applications. The Lab has high- and low-dose radiological facilities, including RPL, PSF–Materials Science and Technology Building (3410), laboratories for thin-film material synthesis and deposition, and the Solid State Lighting Test and Analysis Facility. PNNL works closely with other national laboratories and industrial partners and plays a critical role in high-impact national programs such as JCESR.

The applied materials science and engineering capability forms the basis of PNNL’s sponsor-funded programs in materials synthesis; radiation effects in materials; multiscale behavior of structural materials; modeling, design, and scalable synthesis of materials and chemicals that bridge the mesoscale; fuel cells and energy storage; electric and lightweight vehicle technology; nuclear reactor safety assessment, regulatory criteria, and life extension; and legacy waste forms. These programs are funded through programs in BES, Fusion Energy Sciences (FES), NE, EERE (vehicle technologies, hydrogen storage, building technologies, and fuel cell technology), FE, DOE’s Advanced Research Projects Agency-Energy (ARPA E), EM (waste processing), DoD (materials for storage devices), NNSA, and the U.S. Nuclear Regulatory Commission (NRC).

4. Nuclear and Radiochemistry

PNNL has capabilities in interfacial chemistry, radiochemical separations, analytical measurement techniques, actinides, separations, irradiated materials characterization, spectroscopy, and microscopy. The Laboratory can process and measure plutonium and its fission products across the range of highly radioactive samples in hot cells to ultra-trace measurements of environmental samples in clean rooms. PNNL possesses a unique combination of in-depth knowledge of sample analysis combined with instrumentation, including a focused ion beam and state of the art measurement systems such as the Aberration-Corrected Nuclear Scanning Transmission Electron Microscope (AC Nuclear STEM). Mission-ready instrumentation includes suites of microscopy, mass spectrometric detection, magnetic resonance, and specialized ultra-low-background radiation detectors; numerous specialized wet chemistry laboratories; and ultra-trace radio analytical and radiometric facilities, including a shallow underground lab, providing one of the largest collections of instrumentation and expertise at any single institution in the world.
At the core of PNNL’s nuclear and radiochemistry capability is leadership in plutonium production and waste processing knowledge (specifically in Hanford’s legacy waste), forensic signatures of plutonium production, post irradiation examination of materials, and tritium target fabrication. Staff lead both research and operational programs that make some of the most sensitive measurements of radioactive material in the world and have a track record of maturing scientific breakthroughs into operationally approved methods. This includes development and deployment of the world’s most sensitive radionuclide detection system that operates unattended in worldwide locations and provides monitoring for nuclear tests. The nuclear and radiochemistry capability forms the basis of PNNL’s mission impact in new and improved nuclear detection systems; radioisotope production and advanced instrumentation for nuclear medicine; development of methods and systems to detect nuclear proliferation and combat terrorism; and environmental studies, monitoring, and remediation (for EM).

PNNL stewards a set of facilities unique to the DOE complex. These facilities include Hazard Category II and III nuclear assets such as the RPL. The RPL has the capability to perform an extraordinary range of S&T in a fast and flexible fashion, process materials adjacent to world-class assay technology, and perform testbed scale operation with a wide operational envelope. With the RPL, PNNL can work with micrograms to kilograms of fissionable materials and megacurie activities of other radionuclides. The Physical Sciences Facility complex (3410, 3420, and 3430) houses a wide array of radiochemical processing laboratories and state-of-the-art commercial and custom-designed instrumentation. Programmatic support for nuclear and radiochemistry reaches from scientific discovery (DOE Office of High Energy Physics [HEP], Nuclear Physics [NP], and BES) to research and development (R&D) (NNSA-Defense Nuclear Nonproliferation R&D and DHS-Domestic Nuclear Detection Office) to highly applied programs (EM and DoD-Defense Threat Reduction Agency).

Computational and Mathematical Sciences

5. Advanced Computer Science, Visualization, and Data

PNNL has depth and breadth of expertise in energy-efficient computing; performance, power, and reliability modeling; exploration and design of novel computing architectures; and data-driven discovery at extreme scales. Specific domain areas include programming models, resiliency, fault tolerance, information visualization, data analytics, and data management. Our work is recognized internationally by scientific peers in areas of performance, power and reliability modeling for co-design of systems and applications, design space exploration and optimization, and visual analytics.

Our expertise in programming models for extreme-scale computing is demonstrated through toolkits such as Global Arrays, which powers NWChem and other important scientific applications, including subsurface flow modeling code STOMP and power grid modeling code GridPACKTM. PNNL data scientists lead research in data exploitation, workflow, and provenance at extreme scales for science, energy, and security domains (i.e., the Belle II, ARM, and Cooperative Protection Program efforts). In the field of visual analytics and exploratory data analysis, PNNL has advanced the state-of-the-art in visual metaphors for complex, high-volume data and signature discovery algorithms that apply advanced statistics and machine learning to derive novel indicators for complex phenomena. PNNL is also making significant advances in graph analytics, including hybrid architectures for exploiting large graph datasets and algorithms for scalable graph query on multi-threaded systems.

Special facilities in support of this core capability include the Performance and Architecture Laboratory, a state-of-the-art lab for measuring performance, power, and thermal effects for advanced technologies to predict their overall potential and guide their designs; computing resources, such as the 3.4 petaflop Cascade supercomputer, PNNL Institutional Computing (PIC) mid-range cluster, and research cloud; advanced testbeds for computing technologies, from embedded to extreme; and human-computer interaction research laboratories for visual interfaces, including emerging virtual reality environments.
These resources are housed primarily in the Computational Sciences Facility (CSF) and EMSL. This capability receives support through programs from SC’s Advanced Scientific Computing Research (ASCR), BES, BER, HEP, EERE, FE, NNSA, DHS, and other sponsors, including DHHS and DoD.

6. Computational Science

Computing permeates all research domains at PNNL. The Laboratory actively employs high-performance computing (HPC) to solve compelling, extreme-scale scientific problems, and has a long history of developing computational tools and application codes built collaboratively by multidisciplinary teams composed of domain scientists, computer scientists, and applied mathematicians. PNNL maintains strong capabilities in many computational science domains, including computational chemistry, computational materials science, high energy physics, computational engineering, computational biology, and subsurface science, as well as climate, including participation in developing community climate codes and management of the ARM Climate Research Facility.

Multidisciplinary teams of domain and computer scientists and applied mathematicians have long been an elemental part of the research process at the Lab. For example, as part of developing NWChem, PNNL pioneered engaging teams of computational scientists to create a molecular modeling capability that dramatically advanced the state-of-the-art. This same integrative, co-design-based approach now is being employed to develop advanced computational models for the power grid, high energy physics, materials science, and climate, to name only a few. Moreover, PNNL has been a significant contributor to various DOE Scientific Discovery through Advanced Computing projects.

Internal Laboratory Directed Research and Development (LDRD) investments have focused on bringing together interdisciplinary teams of data scientists, computer scientists, applied mathematicians, applied statisticians, and domain scientists to work on a wide range of DOE-relevant problems in microbiology, soil science, climate sciences, materials, renewable energy, and nonproliferation. Additionally, many PNNL computational scientists have received Innovative and Novel Computational Impact on Theory and Experiment program allocations that span a range of computational science domains. PNNL-developed codes, such as NWChem, are also heavily used on DOE’s Leadership Computing Facility systems and at the National Energy Research Scientific Computing Center.

Staff members are housed primarily in CSF, Information Sciences Buildings 1 and 2 (ISB1 and ISB2), Environmental Technology Building (ETB), and EMSL. This capability leverages support from PNNL’s applied mathematics and advanced computer science, visualization, and data core capabilities and receives support from programs in ASCR, BES, BER, EM, and EERE.

7. Applied Mathematics

PNNL is a leader in applied mathematics and statistics, using mathematical models to predict behavior of complex multiscale systems and quantify associated uncertainty to further scientific discovery. We have a core team of researchers located in ISB1, ISB2, the Biological Sciences Facility (BSF), and CSF that develop novel multiscale methods for uncertainty quantifications (UQs) and data analysis.

PNNL has broad expertise in multiscale mathematics, including dimension reduction, mesoscale Lagrangian particle methods, and hybrid methods for coupling multi-physics models operating at different scales. Building on our strength in multiscale modeling, PNNL is developing capabilities in multi-fidelity methods for parameter estimation and UQ as a part of several projects funded by ASCR, BER, and FE. These techniques focus on solutions for highly nonlinear and high-dimensional systems and include surrogate and multi-fidelity modeling for both forward prediction and inverse models.

PNNL is designing extreme-scale machine learning and data mining algorithms with the Machine Learning Toolkit for Extreme Scale, which includes several supervised learning algorithms (e.g., deep
learning, support vector machine) and unsupervised learning algorithms (e.g., auto-encoders, spectral clustering). Most of the research in data sciences is currently funded by DoD and NNSA.

PNNL also has an emerging capability in the applications of discrete mathematical techniques to a range of problems in the DOE mission space. PNNL leverages these capabilities to solve crosscutting problems of national interest. PNNL is heavily invested in solving issues related to large-scale graph analysis (e.g., data fusion), time evolution of discrete structures, and the development of network invariants and their applications.

8. Cyber and Information Sciences

The Laboratory improves the security and reliability of critical networks and infrastructures through advanced sensing, analysis, and defense, as well as through identifying threats, protecting assets, and detecting, responding, and recovering from incidents. This includes novel information sharing methods and the development and implementation of analytic methods to extract value from data. The research staff are internationally recognized in cyber resiliency theory (encompassing both information and operational technology), cyber analytics, graph theory, semantic computing and knowledge representation, machine learning, text and multimedia analytics, statistics, and human-computer interaction.

PNNL’s cyber security portfolio is based on three decades of expertise in developing and deploying novel cyber security sensors for wide-scale enterprise network monitoring and situational awareness, including operation of the Cooperative Protection Program for DOE-complex cyber defense and the Cyber Security Risk Information Sharing Program, a voluntary information sharing and threat intelligence program for critical infrastructures. PNNL has developed unique expertise in the scientific foundations of cyber security, including leadership in biologically inspired cyber security, multiscale graph methods for active cyber defense, secure supervisory control and data acquisition architectures and communications, critical infrastructure resiliency analysis and modeling, and holistic cyber-physical security.

PNNL’s information science expertise is in areas of data acquisition, management, and storage systems (e.g., data workflow, provenance, and quality assurance); analytics and algorithms (e.g., streaming and graph analytics, scalable machine learning); and decision support (e.g., user experience, real-time analysis, and model/algorithm steering in response to user input). PNNL places special emphasis on developing next-generation techniques for analysis and visualization of unstructured data from heterogeneous sources, including emerging techniques for recommender systems that power new human-machine analytic collaboration.

Major computing resources that support this capability include PIC resources, including the Constance cluster, real-time operating system and scalability testbeds, and the CyberNET virtual enterprise testbed to simulate real world cyber activity and understand blended cyber-physical attacks. In addition, facilities such as the Cyber Innovation and Operations Center, the Electricity Infrastructure Operations Center (EIOC), the cyber-physical PowerNET and CyberNET testbeds, and the Electricity Infrastructure Cyber Security/Resilience Center support this capability. PNNL’s cyber security research staff works closely with the Laboratory’s internal cyber security operations groups, evaluating and deploying analytic and security solutions. External collaborations include industry, academic, and governmental partners from across the nation and around the world. We are united in our pursuit of analyzing, protecting, and ensuring the operations of the nation’s critical cyber infrastructure. Primary sponsors for PNNL’s cyber and information sciences research include ASCR, OE, DoD, and DHS.
9. Decision Science and Analysis

PNNL maintains strong capabilities in modeling, analyzing, communicating, and mitigating crosscutting impacts at the interface between science, technology, policy, and society. Working collaboratively with scientists and engineers across the Laboratory and with external partner organizations, our experts continue to develop and implement innovative, holistic solutions to complex decision problems on the front lines of the nation’s energy and national security challenges.

PNNL’s staff expertise is focused in the areas of decision science, risk analysis, economics, systems engineering, decision support systems, policy analysis, social and behavioral science, statistics, and safety analysis. This capability enables the development and application of cutting-edge decision and risk analysis, safety and risk assessment, making decisions under uncertainty, alternatives analysis, strategic process/systems improvements, and decision support under resource constraints. Additional modeling and analysis capabilities include socioeconomic modeling, market and policy analysis, technoeconomic modeling and analysis, regional/national energy simulation, and cost-benefit analysis and uncertainty analytics. The team’s breadth and depth of decision and risk analysis expertise fosters flexibility in assembling dynamic, multidisciplinary teams to develop science-based strategies for minimizing risks to individuals or the public, program life cycles, facility designs and operations, and the environment at the local, state, regional, national, and global levels.

Staff that support this capability at the Laboratory are located in several locations in Richland, including ISB1, ISB2, the Engineering and Analysis Building, the Math Building, and the National Security Building, as well as the PNNL offices in Portland, Oregon and Seattle, Washington. They are recognized in the areas of nuclear and alternative energy operational safety review and risk assessment; technology field testing, evaluation, and performance assessment; programmatic risk assessment; geo-spatial decision analytics and visualization; nuclear proliferation risk modeling; knowledge management and data reuse; multi-organizational collaboration decision support; distributed decision-making for power grid reliability; energy policy and regulatory development/deployment; appliance and commercial equipment codes and standards; and feasibility analyses of technology, siting, policy, and tax structures for energy technology deployment. Leadership in safety assessment; probabilistic risk assessment methodology development and application; environmental impact assessment; and analyses and feasibility assessments for nuclear, geothermal, hydropower, and other sustainable energy technologies, such as hydrogen-powered vehicles, are specific strengths. Current stakeholders that primarily utilize our capabilities include DOE (EERE, OE, EM, and NE), NNSA, DHS, DoD, the Environmental Protection Agency (EPA), BPA, and NRC.

Earth and Biological Sciences

10. Climate Change Science and Atmospheric Science

PNNL has extensive experience and strengths in measuring, modeling, and understanding the complex interactions among human and natural systems, from molecular to global scales, with expertise spanning the full range of disciplines and tools required to understand atmospheric processes and predict the evolution of the earth’s climate system. This core capability includes activities ranging from laboratory and field measurements to multiscale numerical simulations to integrated analyses of climate impacts and response options. PNNL has domain expertise in atmospheric measurement systems, atmospheric aerosol chemistry, cloud physics and cloud aerosol-precipitation interactions, boundary layer meteorology, land-atmosphere interactions, biogeochemistry, hydrology, ecosystem science, integrated assessment, energy-water nexus, and multiscale atmospheric and earth system modeling. We leverage expertise from related core capabilities, including chemical and molecular sciences; biological systems science; earth system science and engineering; decision science and analysis; power...
systems and electrical engineering; advanced computer science, visualization, and data; and user facilities and advanced instrumentation.

PNNL’s climate change and atmospheric systems research focuses on improving our basic understanding of the causes and consequences of climate change and on developing the data-driven regional and global modeling frameworks needed to predict changes in climate, as well as in related human and environmental systems. Key facilities include the Atmospheric Measurements Laboratory (AML), ARM Climate Research Facility, ARM Aerial Facility, EMSL, Marine Sciences Laboratory (MSL), and Joint Global Change Research Institute (a partnership between PNNL and the University of Maryland focused on understanding the interactions among climate, natural resources, energy production and use, economic activity, and the environment). These facilities house a wide range of world-class equipment, such as a G-1 research aircraft, a flow-through environmental chamber, and wind energy lidar buoys. PNNL is also a leading developer of atmospheric, climate, and earth system models, such as the Global Change Assessment Model, the Weather Research and Forecasting model, DUSTTRAN (DUST TRANsport), and the Accelerated Climate Model for Energy (ACME), as well as in integrating modeling and observational systems across disciplines to yield new insights into the evolution of the coupled human environment system.

PNNL’s capability includes programs in atmospheric-process research, regional and global earth system modeling, integrated assessment, and atmospheric wind energy research. Increasingly, these research activities are being integrated and connected with other research areas and programs (e.g., through integrated multiscale, multi sector modeling that brings together models of climate, hydrology, land surface dynamics, energy systems, and socioeconomics in order to develop more robust understanding of how extreme events and long-term stresses are influencing the energy-water nexus and national security). This core capability is funded by programs in BER, ASCR, EERE (wind and water power technologies), FE (carbon dioxide storage), National Aeronautics and Space Administration (NASA), EPA, and the National Oceanic and Atmospheric Administration (NOAA).

11. Earth Systems Science and Engineering

PNNL’s earth systems science and engineering capability researches the impacts of energy production, storage, and use on valued environmental resources and functions; develops and deploys technologies to mitigate the impacts of past, current, and future energy production systems; and develops and deploys technologies that improve the performance of energy generation and minerals extraction from surface waters. This capability spans terrestrial, aquatic, and coastal ocean systems, both biological and abiotic. Applications of our expertise include Arctic and deep-ocean oil and gas, hydropower, wind power, marine and hydrokinetic generation, algal biomass production, nuclear energy, and legacy waste.

PNNL has scientists and engineers in fields ranging from aquatic and terrestrial ecosystems science, oceanography, biogeochemistry, hydrology, environmental engineering, and microbiology, with domain expertise in molecular-to-field-scale biogeochemistry, laboratory-to-field-scale hydrology, multi-phase flow modeling, integrated (e.g., biogeochemical, physical, ecological) aquatic modeling, aquatic acoustics and tracking technologies, ecosystem-level adaptive management, biofouling/bio-corrosion, climate-simulating culturing of algae and higher plants, minerals extraction from seawater, ecosystems modeling and restoration, human health and environmental risk assessment, and environmental systems technology development and deployment.

PNNL is home to the only marine research facility in the DOE complex, the MSL in Sequim, Washington. MSL’s coastal location and facilities enable studies of anthropogenic impacts on marine species and systems; a controlled study area for development and testing of marine energy systems; biogeochemical, ecotoxicological, and biotechnology investigations with ambient seawater; and a platform for development and testing of autonomous and in situ marine technologies. In addition,
PNNL’s distinctive Aquatics Research Laboratory supports fisheries research focused on sustainable hydropower operations and development. Advanced environmental monitors and ecological sensors for conventional hydropower, wind, marine, and hydrokinetic renewable energy systems are developed and tested at PNNL’s Bio-Acoustics and Flow Laboratory (LSL II). The advanced experimental and instrument capabilities of EMSL are also used to advance research in this area.

PNNL conducts research at the bench, pilot, and field scale, integrated with advanced modeling and simulation, to provide the technical underpinnings, scientific approaches, and technological advancements to support breakthrough solutions, improve system knowledge, and champion new protocols that are protective of human health and the environment. The earth systems science and engineering capability is funded through programs in BER, BES, EM, NE, EERE, NRC, EPA, DHS, Department of Interior, NOAA, and the U.S. Army Corps of Engineers.

12. Environmental Subsurface Science

PNNL’s environmental subsurface science capability focuses on developing and applying knowledge of fundamental biogeochemical reactions, energy, and mass transfer processes to the prediction and assessment of natural processes, including the natural attenuation of contaminant plumes and engineered systems, such as the design and operation of carbon sequestration reservoirs. PNNL provides DOE with domain expertise in molecular through-field-scale biogeochemistry, reactive transport modeling, lab-to-field-scale geohydrology, multi-phase flow modeling, computational geochemistry, subsurface technology development and deployment, advanced geophysical monitoring, isotopic analytical capabilities, and high temperature and pressure geochemistry. Potential applications include enhanced oil recovery, geologic carbon storage, geothermal energy development, and technology development for deep borehole nuclear waste repositories.

For EM, PNNL applies an integrated experimental and modeling approach to resolve technical issues necessary to inform decisions for environmental remediation, waste management, and closure. PNNL has teamed with other laboratories to develop the Advanced Simulation Capability, a state-of-the-art scientific approach that uses integrated toolsets for understanding and predicting contaminant fate and transport in natural and engineered systems. PNNL leads the Deep Vadose Zone-Applied Field Research initiative, providing the technical basis to quantify, mitigate, and monitor natural and post-remediation contaminant discharge from the vadose zone to groundwater. Outcomes include advanced prediction, characterization, remediation, and monitoring approaches for addressing residual soil and groundwater contamination at DOE facilities, as well as the protection of regional water resources and aquatic ecosystems.

This capability is also applied to numerous energy and water challenges, including sustainable energy generation, production, and use resulting in PNNL emerging as a national leader in geologic sequestration science. Through the Big Sky Carbon Sequestration Partnership, PNNL led one of the world’s first carbon storage projects into basalt formations, completing a 1,000 ton injection into the Grande Rhonde basalt formation. PNNL has key roles in FE’s National Risk Assessment Partnership, leading the Groundwater Protection Focus Area. Through its BER-funded Science Focus Area, PNNL is leading research in molecular and microscopic electron transfer processes, pore-scale reactive transport and upscaling, and field-scale microbial ecology and biogeochemistry. Staff members support programs funded by BER, BES, EM, FE, EERE (Geothermal Technologies Office), NRC, NNSA, DHS, EPA, NASA, and DoD, as well as DOE’s emerging integrated program in Subsurface Technology and Engineering Research, Development, and Demonstration Crosscut. Staff and capabilities are located across the PNNL campus in Richland and Sequim facilities including: EMSL, LSL I, LSL II, ISB2, ETB, and MSL.
13. Biological Systems Science

Through PNNL’s biological systems science core capability, the Lab is developing a mechanistic understanding of complex multicellular systems and their response to perturbation to enable improved predictions of the impacts of climate, energy production, and emerging technologies on environmental sustainability and human health.

PNNL has made significant contributions in deciphering mechanisms of microbial community metabolic interactions and dynamics, understanding multiscale terrestrial biogeochemistry, predicting contaminant behavior and microbial ecology of the subsurface, quantifying the effects of renewable energy devices on aquatic ecosystems, and applying a systems biology approach to plant, microbial, and algal systems relevant to DOE’s missions in science, energy, and environment. In addition, the “Microbiomes in Transition (MinT)” LDRD investment leverages the strengths within this core capability, biological and bioprocess engineering and earth systems science and engineering, to understand the metabolic activities of complex microbial communities and how metagenomes translate to the function of a microbial community, as well as to illuminate the microbiome’s role in plant and animal and human health, biogeochemical cycling, and impacts on climate. PNNL’s expertise in fungal biology has generated an in-depth understanding of the biological processes underlying efficient fungal bioprocesses that produce fuels and other chemicals. In addition, PNNL is providing insight into the development of medical countermeasures, early diagnostics, biodetection, and bioforensics to improve health and biosecurity.

In combination with other core capabilities, including chemical and molecular sciences; environmental subsurface science; advanced computer science, visualization, and data; applied mathematics; and large-scale user facilities/advanced instrumentation, this core capability delivers expertise in microbial ecology, microbiome science, fungal biology and biotechnology, pathogen biology and biological threat analytics, systems toxicology, plant science, biochemistry and structural biology, trace chemical analysis, biomolecular separations, advanced in situ and dynamic imaging, computational biology and biophysics, and signature discovery through data analytics. PNNL’s integrative ‘omics capabilities, widely used by the BER programs (e.g., the mechanisms of metabolic exchange among members of microbial communities), leverage this broad suite of expertise to provide unprecedented molecular- to mesoscale resolution of the structure and activity of biological systems.

This capability is funded through programs in BER, ASCR, BES, EERE, EM, DHS’s Science and Technology, DoD, NIH, NASA, and the EPA. Key facilities supporting this capability include BSF; CSF; the Bioproducts, Sciences, and Engineering Laboratory; MSL; the Aquatic Research Laboratory; LSL I; Microbial Cell Dynamics Laboratory; and EMSL. PNNL partners with the Joint Genome Institute (JGI) to provide large-scale genome sequencing and analysis for DOE missions. EMSL and JGI now issue an annual joint call for user projects focused on synergistic use of capabilities at both facilities, targeting collaborative science projects in biogeochemistry, carbon cycling, and biofuels.

Engineering

14. Biological and Bioprocess Engineering

PNNL is developing technologies and processes to convert biomass and waste materials into fuels and chemicals that will reduce the United States’ dependence on petroleum. Biomass sources include lignocellulosic materials (e.g., corn stover and wood wastes) and other waste materials (e.g., waste water treatment plant wastes), as well as algae. Decades of research have established biological and bioprocess engineering as a PNNL core capability. This capability leverages expertise in catalysis and reaction engineering, separations, process engineering and flowsheet development, materials science, and techno-economic modeling. Research spans from understanding the molecular interactions involved
in the conversion processes to pilot-scale operations that demonstrate technologies, allowing them to be transferred to industry for commercial application.

PNNL’s biologists, chemists, and chemical engineers specialize in fermentation, algae growth and processing, catalysis and reaction engineering, separations, process engineering, techno-economic and lifecycle analyses, and resource assessments. Staff members are housed in our Bioproducts, Sciences, and Engineering Laboratory and MSL to solve the most challenging bioprocessing issues. PNNL’s technical areas of expertise include fast pyrolysis for converting biomass to bio-oil, hydrothermal liquefaction for conversion of wet materials to products, hydrotreating of biocrude and bio-oils to fuels, conversion of biomass-generated alcohols to jet fuels (validated by both the Air Force and industry), and conversion of intermediates to chemical products. PNNL houses unique indoor, climate-controlled raceway ponds that can cultivate microalgae strains under conditions that simulate outdoor ponds at any geographic location in the world. We also utilize a unique Biomass Assessment tool used by the government and industry to quantify potential fuel production from microalgae and waste feedstocks. This capability maintains a portfolio with significant intellectual property (IP) that enables commercialization of DOE and other investments. The PNNL team has seven distinguished inventors, each with 14 or more awarded U.S. patents, for a total of 65 bio-based U.S. patents since the year 2000. This capability supports other PNNL core capabilities, including biological systems science, chemical engineering, applied materials science and engineering, chemical and molecular sciences, and earth systems science and engineering. PNNL provides leadership in biological and bioprocess engineering to the EERE Bioenergy Technologies Office, EM, academia, and industry. Industrial partners include companies such as Archer Daniels Midland, Genifuel, and LanzaTech.

15. Power Systems and Electrical Engineering

PNNL has domain expertise in the power grid’s conventional and variable generation, transmission system, distribution network, smart grid with demand response, market systems, and energy demand areas. PNNL experts develop innovative solutions to addressing emerging challenges facing today’s power industry, by better planning, operating, and controlling the modern power grids for enhanced resiliency and reliability. Primary supporting disciplines include power systems and electrical engineering, computational science, and mechanical engineering. With a focus on system-level issues, PNNL is the national leader in defining the inherently resilient power grid of the 21st century, delivering innovative tools to enable unparalleled grid performance (reliability, security, efficiency, and sustainability) and new control and architecture paradigms spanning future demand and supply for unprecedented consumer engagement.

PNNL is specifically known for its expertise in power grid research, with power systems and electrical engineering researchers, computing, and data experts. Key research areas include grid architecture, transmission and distribution system reliability and control analysis, power system protection, advanced grid data, computing and visual analytics, renewable integration, energy storage, distribution system modeling, and grid cyber security. This expertise in grid simulation and analytics enables high-performance grid monitoring and control at unprecedented speed, from minutes to sub-seconds. For over a decade, PNNL has led the world in the development and applications of transactive systems that combine economics and controls to enable distributed optimization and integration of distributed energy resources including responsive loads, batteries, and renewable resources. PNNL’s expertise in advanced control theory, application, and testbeds supports advances in the development of new, distributed controls for the electric power system. PNNL’s leadership in phasor measurement technologies supports broader national deployment, enabling unprecedented grid visibility and enhanced situational awareness. One-of-a-kind, utility-grade control center infrastructure supports research in grid visibility, control, and resiliency, with the largest national repository of grid data and models to inform research.
This research is made possible with the use of the EIOC, Interoperability Laboratory, Power Electronics Laboratory, and the Electricity Infrastructure Cyber Security/Resilience Center in the Systems Engineering Building (SEB). These laboratories and facilities support world-class commercial tools, as well as the GridLAB D™ simulation and analysis tool for designing and operating power distribution systems, the GridAPPS D open source platform for advanced distribution system planning and operations application development, the GridPACK package for parallelizing power grid simulations, the VOLTTRON™ software platform enabling smart appliances, the Dynamic Contingency Analysis Tool (DCAT) for enabling power grid cascading failure analysis, electric vehicle charging, and the ramping tool for assessing power grid ramping capabilities with increased variable generation. These capabilities are funded through programs in OE, EERE (transportation technologies, hydrogen storage, building technologies, and fuel cell technology), ARPA-E, DHS, ASCR, DoD, the U.S. Department of State, and private industry.

16. Systems Engineering and Integration

PNNL is recognized for systems engineering and integration through the implementation of technology in real world complex systems, focusing on smart and robust energy and nuclear material security. This core capability has solved some of the most challenging national problems by defining and interpreting complex technical requirements and translating them into fieldable solutions that address economic, social, policy, and engineering considerations. Using a structured approach to understand complex systems throughout their lifecycle, PNNL applies its domain knowledge and experience in engineered systems simulation and modeling; system architecture and design; test, evaluation, and optimization; technology assessment, integration, and deployment; policy assessment and economic evaluation; and regulatory analysis, risk assessment, and decision support. This allows our staff to effectively take early-stage research through the development and technology maturation processes and to deploy technical solutions that address our sponsor’s most critical challenges.

PNNL applies a graded approach to our systems engineering discipline that enables us to deliver solutions in a highly efficient, effective way. PNNL is known worldwide for field-deploying international nuclear materials safeguards, security, and complex radiation detection systems. PNNL also is developing integrated building energy technologies, advancing national power grid reliability and smart grid technology, and conducting large-scale technology demonstrations. Staff members are housed in facilities that include SEB, the Electrical Infrastructure Operations Center, System Engineering Facility, 2400 Stevens, Engineering Development Laboratory, Applied Processes and Engineering Laboratory, Radiation Detection Laboratory, and the Large Detector Test Facilities.

The systems engineering and integration capability is funded through programs in BES (design and operation facilities), BER, HEP, NP, EERE (buildings and transportation), EM (waste processing and nuclear materials disposition), OE (infrastructure security and energy restoration), FE (carbon- and co-sequestration), NNSA (nonproliferation and safeguards), DHS (radiation portal monitoring and critical infrastructure and analysis), NRC, EPA, and DoD.

17. Chemical Engineering

PNNL’s chemical engineering capabilities translate scientific discovery into innovative, first-of-a-kind processes to solve the nation’s toughest energy and environmental challenges. PNNL develops materials, unit operations, and chemical processes at scales ranging from molecular interactions to engineering-scale experiments, through full-scale demonstrations that can be transferred to the sponsor or to industry for commercialization. PNNL has chemical engineers, mechanical engineers, and chemists specializing in disciplines including catalysis and reaction engineering, gas and liquid phase separations, heat exchange, process intensification, fluid dynamics and mixing, thermal-mechanical modeling, flowsheet development and modeling, and techno-economic analyses. Other distinctive areas of
expertise include radioactive and non-radioactive nuclear waste treatment (from milligram to ton-scale), encompassing slurry transport and mixing, glass melting, advanced rheology, and fluid dynamics for complex multi-phase systems.

PNNL applies chemical engineering capabilities to a broad array of challenges and successes. Successes include the development and commercialization of NOx reduction units for automobile emissions control, leading the development and application of software to predict the thermal and structural performance of spent nuclear fuel storage and transportation systems, development of novel heat pumps and building systems to increase energy efficiency, and invention and development of micro-technology-based reactors and separations systems for applications such as fuel cells and solar natural gas reforming. Current focus areas include biomass and fossil fuel conversion to fuels and chemicals, as well as subsequent fuel upgrading; nuclear waste processing and immobilization research to solve the nation’s legacy nuclear waste challenges; and cost-effective startup and operation of the Hanford Waste Treatment Plant.

This core capability supports other PNNL core capabilities in applied materials science and engineering, biological and bioprocess engineering, chemical and molecular sciences, nuclear engineering, and systems engineering and integration. This capability supports sponsor-funded research by SC (BES), EM, EERE (Vehicle Technologies Office, Bioenergy Technologies Office, Geothermal Technologies Office, Solar Energy Technologies Office, and Fuel Cell Technologies Office), FE, NE, NNSA, ARPA-E, and DoD.

18. Nuclear Engineering

PNNL has expertise in complex irradiation systems that support materials science, tritium production, advanced fuel modeling, and reactor production analysis. Research staff members have a broad and deep technical skill set across the full spectrum of nuclear engineering disciplines, including reactor physics, mechanical design, thermal-mechanical analysis, fluid dynamics, heat transfer and criticality safety, nondestructive evaluation, and robotics, as well as materials science and microscopy. A strong knowledge base and expertise in commercial nuclear industry enables design of targets for isotope production and fuel performance modeling to develop or evaluate fuels for use in NRC-regulated commercial or research reactors.

PNNL is specifically recognized for the development of the Graphite Ratio Method, which is the world’s most accurate estimation tool for graphite reactor operational history, and has a deep expertise in proliferant plutonium production, from reactor to plutonium metal. PNNL is the design authority for tritium production targets used in a commercial reactor and is noted for expertise in remote sensor design to enable reactor life-extensions. The combination of thermal, nuclear, and structural skills is also used to evaluate spent nuclear fuel storage and transportation options. PNNL staff members have a unique understanding of international nuclear capabilities and, thus, the ability to assess all source information.

PNNL is able to apply these skills in radiological facilities (e.g., the RPL) to characterize and understand irradiation effects on materials through post-irradiation examination and to make precise measurements and analysis that enable nuclear archeological assessments. In addition, PNNL has experimental testing capabilities that enable design, development, and fabrication of advanced, accident-tolerant fuel for commercial reactors and low enrichment fuel for research reactors, as well as design, modeling, fabrication, and deployment of complex irradiation tests to evaluate nuclear materials. The nuclear engineering capability is funded through programs in the BES, HEP, NP, EERE, EM, NNSA Defense Programs, NE, DoD, DHS, EPA, and NRC.
19. User Facilities/Advanced Instrumentation

EMSL is a BER scientific user facility that is pioneering molecular-level discoveries to enable the predictive understanding that will provide the foundation for critical biological, environmental, and energy challenges. EMSL accomplishes its mission through four transformational science themes: 1) atmospheric aerosol systems, 2) biosystem dynamics and design, 3) terrestrial and subsurface ecosystems, and 4) the new molecular transformations theme, which replaces energy materials and processes. Multidisciplinary teams of users working on these themes collaborate with EMSL’s expert staff and use instrumentation and computation within EMSL to solve complex scientific problems. EMSL provides scientific leadership and access to instrumentation in high performance mass spectrometry (MS), high-resolution microscopy, high-field magnetic resonance spectroscopy and imaging, surface and interface spectroscopies, sophisticated biological characterization techniques, and high-performance molecular science computing, all unmatched in sensitivity and resolution, sample throughput, and variety of in situ sample environments.

PNNL is recognized for its ability to conceive, design, build, operate, and manage world-class scientific user facilities and is known internationally for its advanced instrumentation designed to accelerate scientific discovery and innovation. As an example, PNNL recently demonstrated this ability with the development, design, construction, and operation of the 21-Tesla Fourier-Transform Ion Cyclotron Resonance (FTICR) MS.

This capability also enables PNNL’s contribution to the design and operation of the ARM Climate Research Facility. ARM is the world’s premier ground-based observational facility for advancing climate change research, used by scientists worldwide to improve the understanding and representation of clouds, aerosols, and other key processes in climate and earth system models. Providing a global network of instrumented fixed, mobile, and aerial observatories for obtaining cloud and aerosol measurements, as well as precipitation, solar and thermal radiation, surface heat and moisture, and meteorological conditions, ARM observation sites are in climate-critical regions such as the eastern North Atlantic, Antarctica, and the north slope of Alaska. To support model development and associated atmospheric-process studies, ARM has developed a mega-site in the Southern Great Plains that will provide three-dimensional constraints to high-resolution model simulations. PNNL is responsible for the overall technical direction of ARM’s scientific infrastructure through continual collaboration among nine DOE laboratories.

This capability is funded by SC (BER, ASCR, BES, and HEP), EERE, DHS, and NIH-National Institute for General Medical Sciences.

Science Strategy for the Future

PNNL, as the nation’s premier chemistry, earth science, and data analytics laboratory, conducts world-leading research and development to address our most challenging problems in energy resiliency and national security. Our leadership in chemistry is advancing the scientific community’s understanding of catalytic reaction mechanisms, and delivers the science and technology needed to enable secure and flexible electric and energy systems. The focus we have in earth systems sciences on the understanding of clouds and aerosols, the water and carbon cycles, and the emergent behavior of microbial communities provides a fundamental scientific foundation for our work to improve human, plant, and animal health; remediate the environment; produce bio-based fuels; and understand the environmental impact of energy systems. Our strengths in measurement sciences and data analytics provide us with a deeper understanding of radiation dynamics for nuclear security and environmental restoration, as well as the expertise to develop complex signatures for real-time cyber-enabled systems.
Major Initiatives

PNNL has six major initiatives that are designed to deepen and broaden our science base while enabling critical mission outcomes in energy resiliency and national security. Similar to the stewardship of our core capabilities, advancements in our major initiatives are largely funded by our sponsors. In addition, PNNL’s LDRD portfolio is designed to support and enhance our major initiatives.

We have investments designed to deepen our existing world-class capabilities in catalysis and materials science and to answer fundamental questions related to how the structures and properties of materials in radioactive environments evolve with time. In addition, we are working toward developing the mathematical basis for new control theories, a critical need for a secure and resilient electric grid. PNNL’s FY 2018 LDRD investments include multiyear efforts on topics that range from use-inspired development of carbon-neutral chemical conversion techniques to discovering how the microbiome behaves under changing conditions to developing algorithms relevant to processing streaming data at speeds and scales currently unfeasible.

Each of our major initiatives has both sponsor funding and LDRD investments to accelerate the rate of innovation, leading to significant scientific advancements, technological breakthroughs, and new strategic partnerships with other research organizations. Each initiative draws upon a subset of our core capabilities and provides a focus for evolution of those capabilities into the future.

Infrastructure

Site Facilities and Infrastructure

PNNL is located in southeastern Washington State, in the city of Richland, with buildings on the Laboratory’s main campus and on the Hanford Site. PNNL also conducts operations at the MSL in Sequim, Washington. Specifically, PNNL consists of

- 21 DOE-owned buildings—9 owned by EM and 12 owned by SC (874,346 gsf; average age 27 years)—and 18 OSFs
- 29 Battelle-owned buildings (473,088 gsf; average age 45 years) and 23 OSFs on 203 acres, including 39 acres in Sequim
- 27 buildings from third-party leases and agreements (962,119 gsf; average age 24 years).

As part of the PNNL contract, Battelle has provided DOE with exclusive use of the Battelle-owned facilities for PNNL purposes. Battelle facilities comprise 23 percent of the PNNL laboratory space and are provided to the government at cost. DOE and Battelle have reached contractual agreement to transfer the Battelle-owned Richland and Sequim, WA facilities to DOE upon the buildings’ full depreciation on or before the end of FY 2022.

PNNL’s non-federal-owned space is evaluated for operational efficiency, consolidation, and/or reduction opportunities. In FY 2016, PNNL extended seven leases, terminated one lease, added two leases, and changed square footage on three leased buildings. A summary of PNNL’s actual FY 2016 and planned FY 2017 real estate actions, including new (or renewal) leases > 10,000 square feet, can be found at the following website: http://www.pnnl.gov/campusplan/lab_plan_real_estate_actions_schedule.pdf. In FY 2017, we are not planning any disposals of DOE land via leasing, sale, or gift within the planning horizon.

The utility infrastructure and distribution systems that serve PNNL’s Richland Campus, the MSL, and PNNL operated buildings in the Hanford 300 Area include roads, electricity, water, sewer, gas, storm drain, telephone, and telecommunications. Generally, the utility infrastructure and distribution systems are in adequate condition and have the necessary capacity to meet current mission needs. The service providers for the various utility infrastructure and distribution systems include EM contractors, Battelle
as PNNL’s operating contractor, the City of Richland, and the City of Sequim. We are currently evaluating options for changing service providers based on long-term value to PNNL operations.

The FY 2016 condition and utilization assessment designated all of the federally-owned, active, operating buildings and trailers as adequate relative to mission. Of the 21 buildings and trailers, 19 are fully utilized. A majority of non-federally-owned, active, operating buildings and trailers were designated as adequate relative to mission (52 of 56) and fully utilized (47 of 56) in the FY 2016 condition and utilization assessment. None of the assets were designated inadequate relative to mission or not utilized. Actions to resolve the underutilized buildings and trailers, and the substandard assets relative to mission and/or underutilized buildings and trailers are described in section 6.2, Campus Strategy.

**Campus Strategy**

PNNL is implementing a rolling, 10-year campus strategy designed to deliver the foundation for the multidisciplinary science and engineering expertise, equipment, instrumentation, facilities, and infrastructure required to enable the science strategy and scientific vision discussed in sections 3.0 and 4.0. We continue to make proactive investments to acquire new and/or renew our existing facility and infrastructure assets for long term value and adaptability that support the following objectives:

- Deliver current and future mission alignment by providing the physical environment that meets current and emerging research needs required to deliver vital mission impacts in energy resiliency and national security
- Optimize the functionality, reliability, utilization, and operating costs of our facility and infrastructure capabilities to enable research operations.
- The investments must also:
  - Embrace our guiding principles for developing a modern, collaborative, flexible, and sustainable campus by providing or incorporating:
    - state-of-the-art space and infrastructure to promote creativity, develop technical leaders, and encourage staff members to be bold in their research
    - a connected campus to enable institutional and individual collaborations and research operations that accelerate high-impact research
    - flexibility in design and space use to rapidly respond to changing research needs
    - consideration for environmental, social, and economic costs in the design, construction, allocation, and use of space to optimize energy and materials usage while enabling research.
- Balance our intentions for long-term value from a mission-aligned, functional, reliable, fully-utilized, modern, collaborative, flexible, and sustainable campus with what is reasonable and achievable given available time, investment, and operational resources.

Successful execution of the campus strategy has resulted in the following accomplishments:

- Exit 16 buildings (8 Battelle and 8 leased), reducing our facility footprint by more than 166,000 gsf and operational costs by more than $3M annually.
- Three new federal buildings—3820 (SEB), 3850 (General Purpose Chemistry Laboratory [GPCL]), and 3860 (an office building)—will be completed by 2017 fiscal year-end.
- Relocated radiological and non-radiological work from the Research Technology Laboratory (RTL) complex in preparation for decontamination and decommissioning actions to reduce DOE risk from past radiological operations in facilities that are now adjacent to residential development.

In FY 2017, EM and SC signed a Memorandum of Agreement for the administrative reassignment of 85.6 acres of Hanford Site Land from EM to SC. This change was documented in the Facilities Information Management System (FIMS) in January 2017.
Figure 2 shows PNNL’s campus strategy site map at the end of FY 2028, with ownership, new construction, and exit of non-DOE buildings. Over the next 12 years (starting in FY 2017), we plan to invest $296M to build up to eight new federal buildings totaling ~140,000 gsf, exit up to ~196,000 gsf, and modernize and sustain existing, retained buildings and infrastructure. In addition, we are developing the project documentation to support $112M in direct funding for three new federal buildings totaling ~117,000 gsf. The new federal buildings and consolidating existing space will replace the exited space.

Our investment plans and actions for delivering a mission-ready campus aligned with our campus strategy objectives are summarized below. The plans and actions are based on our annual evaluation of current space utilization and mission projections. Investments by core capability are shown in Table 4. Funding for the campus strategy includes internal, infrastructure, and general plant project investment. The type, timing, and alignment of the investments to our campus strategy objectives are summarized in Table 5. Table 6 shows the Integrated Facilities and Infrastructure Crosscut data per the Integrated Facilities and Infrastructure Guidance definitions.

**Mission Aligned.** The ESC is proposed to be funded by SC to fill the gaps identified in section 4.2.1 and the approved mission need statement and to deliver the desired end-state with the required integration and collaboration, which will provide the following.

- Accelerated scientific discovery by close integration of unique, dynamic characterization capabilities with synthesis and computation capabilities.
- Ability to transfer samples *in situ*, which our current capabilities do not allow, ensuring sample integrity when moving from one station to the next.
- Rapid advances in computational architectures and software through co-design by synergistic mapping of domain science, algorithms, tools, and computer science.
- Development of exascale computational tools that will transform our ability to predict and design catalytic processes.
- Space in EMSL for expansion of plant and soil science capabilities, including capabilities focused on aerosol life cycle, soil science, hydro-biogeochemical cycling, and plant science currently housed outside of EMSL, thus increasing utilization of EMSL capabilities and enhancing the availability of these capabilities to EMSL’s users.

There is a shortage of appropriate high-bay space at PNNL (the existing 36,000 square feet is 99 percent utilized). The Thermochemical Processing Facility is proposed to be funded by EERE. This proposed investment will address the need to relocate away from public encroachment, and will use a purpose-built design for the hazards, constrained ability to perform concurrent operations, and the ability to consolidate operations requiring high-bay space tailored to these program-specific needs.

The Hydropower Engineering Facility is proposed to be funded by EERE. This proposed investment will provide high-bay research and engineering space to improve the performance of fish passage through hydropower turbines, hydrokinetic devices, and related structures, and will test and validate those water power technologies at several readiness levels.

A new, Institutional General Plant Projects (IGPP)-funded, federally-owned, collaboration building called the Collaboration Facility started construction in FY 2017. Completion and operational startup are scheduled for FY 2018. This facility will increase researcher effectiveness and scientific innovation. The building provides new, flexible space for S&T collaboration, food services, meeting spaces, and improved arrival services by consolidating point-of-entry activities and decreasing onboarding time for visitors, interns, and new hires, making it a positive experience that quickly transitions personnel to the purpose of their arrival.
Figure 2 - PNNL 10-year campus strategy site map showing land ownership, PNNL Richland campus area, new construction, and non-DOE building exits planned/completed (new construction building locations are notional)
An internally funded project to reduce the current insufficient, ventilation-intensive, wet, radiochemistry space condition is underway. Project scope includes relocating non-radiochemistry work from 3420 and 331 and modifying 3420 space for additional radiochemistry labs.

**Optimize Functionality, Reliability, Utilization, and Operating Costs.** We plan to invest in both new and existing facilities and infrastructure assets to optimize campus functionality, reliability, and utilization to improve research operations while maintaining or reducing operating costs. This approach is particularly important at PNNL given the mix of federal and non-federal assets. Over the next 10 years, investments to replace and/or consolidate non-federal land, office, high-bay, and laboratory space into federal land and space include the following:

- DOE and Battelle have reached contractual agreement to transfer the Battelle-owned Richland and Sequim, WA facilities to DOE upon the buildings’ full depreciation on or before the end of FY 2022. DOE and Battelle have also agreed that DOE has the right to acquire or lease Battelle-owned land in Richland and Sequim, Washington, and DOE has agreed to fully exercise this right on or before the end of FY 2035, subject to the availability of funds. This agreement results in DOE acquiring 21 Battelle-owned buildings and approximately 247 acres in Richland and Sequim, Washington. Capital investments related to this agreement are included in Table 5.

- We will construct office and lab buildings needed to support exits from non-federal facilities in the FY 2024 to FY 2028 timeframe.

We have undertaken a facilities restoration program to retire SC’s current liability associated with the historical use of radiological and other materials in Battelle-owned buildings. The program will characterize and remediate the buildings as required to achieve unrestricted release, scheduled for completion in FY 2017. One specific building, RTL 520, has known contamination (e.g., beryllium, radiological, and other) and has residential development within 440 feet. The strategy includes PNNL internal investments to deactivate, decommission, decontaminate, and demolish RTL 520 and the RTL outbuildings.

Below are examples of where we are investing internal resources to optimize the campus functionality, reliability, and utilization while maintaining or reducing operating costs.

- Replace acid-degraded hoods and end-of-life utilities and building systems that will improve capabilities for handling radiological materials.

- Continue to invest in the necessary maintenance and repair to maintain our retained assets in a mission-ready condition aligned with our campus strategy objectives. Our current deferred maintenance in SC facilities stands at $0M.

- Address a portion of the underutilized and substandard basement in LSL II, a 102,107 gsf building, by modifying the ventilation stack system; converting vivarium laboratory spaces into functional, general purpose, wet laboratories; and relocating compatible work from non-federal facilities.

- Continue actions to drive better utilization of our mission-unique, Hazard Category II nuclear facility through investments in staff and equipment to enhance the overall facility capabilities. Examples include providing quiet space capabilities, replacing an end-of-life process chiller, and replacing acid-degraded fume hoods to avoid potential failures in the ventilation system. Implementing a carefully planned project to increase the accountable nuclear material inventory limits is needed to reduce impacts to research and reduce the risk of exceeding the existing limit.
- Relocate capabilities to the new ESC building, modernizing and backfilling the exited spaces to increase functionality, utilization, and collaboration across the campus and reduce operating costs.

- Resolve ventilation system capacity issues between BSF and CSF to increase system reliability.

- Resolve an ongoing need for outdoor testbed space for conducting large-scale experiments.
LABORATORY

Lab-at-a-Glance

- **Location**: Princeton, NJ
- **Type**: Single-program Laboratory
- **Contractor**: Princeton University
- **Site Office**: Princeton Site Office
- **Website**: www.pppl.gov

**Physical Assets:**
- 91 acres and 30 buildings
- 765k GSF in buildings
- Replacement Plant Value: $660M

**Human Capital:**
- 3206 Full Time Equivalent Employees (FTEs)
- 256 Joint Faculty
- 268 Postdoctoral Researchers
- 322 Graduate Students
- 260 Undergraduate Students
- 7,422 Facility Users
- 1,005 Visiting Scientists

**FY 2016 Costs by Funding Source ($M)**

- **FES**: $83.2
- **BES**: $1.4
- **SPP**: $2.1
- **Other SC**: $5.5
- **NNSA**: $0.8
- **Other SC**: $5.5

Mission Overview

The Princeton Plasma Physics Laboratory (PPPL) is an innovative and discovery leader in plasma and fusion science and engineering. It is the only Department of Energy (DOE) Laboratory devoted to these areas, and it is the lead U.S. institution investigating the science of magnetic fusion energy.

For over six decades PPPL has been a world leader in magnetic confinement experiments and nationally leading programs in plasma theory and computation, and plasma science and technology. PPPL is a partner in the U.S. contributions to the international ITER Project and hosts multi-institutional collaborative work on the National Spherical Torus Experiment – Upgrade (NSTX-U) facility. The Laboratory also hosts smaller experimental facilities used by multi-institutional research teams and collaborates strongly by sending scientists, engineers, and specialized equipment to other research facilities in the U.S. and abroad.

In FY2018, one of our highest priorities is to rebuild NSTX-U into a robust and reliable SC user facility. In addition, PPPL will address issues in several functional areas: quality assurance/control, contractor assurance, engineering practices, training and qualification, and project management. Most of our twelve management systems will be impacted by the implementation of the institutional corrective action plan.

The Laboratory has two coupled missions.
• First, PPPL develops the scientific understanding of plasmas from nano- to astrophysical-scale. Plasma physics, the study of hot ionized gas, is crucial to understanding the dynamics of the visible universe and solar system, and high-temperature matter in all contexts. This knowledge has a broad range of applications, including fusion energy, forecasting the impact of solar storms, semiconductor chip manufacturing, and technological development (e.g., plasma production of carbon nanotubes).

• Second, PPPL develops the scientific knowledge to enable fusion to power the U.S. and the world. Under appropriate conditions and composition, plasma with very high temperature, density, and confinement will release energy from nuclear fusion. PPPL has been a leader in developing the physics understanding of high-temperature plasmas needed for fusion. PPPL will continue to solve plasma physics problems crucial to fusion energy, as well as contribute to solutions of key engineering science challenges associated with the material structure that surrounds the hot plasma.

Woven throughout PPPL’s approach, as a core part of Princeton University’s culture, PPPL educates and inspires future generations for the national interest. This includes outreach programs for science education from grammar school to college, a world-leading graduate education program in plasmas and astrophysical sciences in conjunction with Princeton University, and hosting hundreds of external students and thousands of visitors each year.

Core Capabilities

As a pioneer with decades of contributions to the U.S. and international fusion and plasma physics research communities, PPPL possesses core capabilities vital to the DOE Office of Science’s mission to develop the knowledge base for fusion energy and high-temperature plasmas. These capabilities include Plasma and Fusion Energy Sciences, Large Scale User Facilities/Advanced Instrumentation, Mechanical Design and Engineering, Power Systems and Electrical Engineering, and Systems Engineering and Integration. Lapses in the last four of these have prompted actions by the Laboratory to strengthen its Engineering organization under new leadership and to implement reforms in its procedures intended to restore the required degree of rigor in its engineering activities.

The series of reviews flowing from NSTX-U technical failures, culminating in a June-August 2017 external Extent of Cause review, have served to identify needed Laboratory-wide corrective actions. PPPL is taking aggressive action to implement near-term recommendations from this review. Early activities to be completed by the onset of FY2018 include the assignment of an accomplished Project Manager to lead the NSTX-U Recovery Project and PPPL performance improvement campaign and to make foundational improvements to PPPL’s Quality Assurance (QA) Program and key engineering procedures. Throughout FY2018 PPPL will draw upon University and external assistance from across the DOE complex in making substantial changes to management systems with the goal of transforming Laboratory performance. To

While the main focus of PPPL’s capabilities is the research by Fusion Energy Science (missions SC 17-20), they also support other important DOE missions and receive supplementary funding from Advanced Scientific Computing Research (mission areas SC 1, 3, 6), Basic Energy Sciences (mission area SC 7), High Energy Physics (mission area SC 25), and the National Nuclear Security Administration (NNSA). In FY2018, the Laboratory and the University will also address skill-mix gaps in our current workforce to complete the NSTX-U recovery project, improve efficiency and effectiveness across the laboratory, and increase facility maintenance spending to improve the Laboratory infrastructure.

1. Plasma and Fusion Energy Sciences
PPPL offers world-leading experimental and theoretical capabilities and facilities to explore the physical processes that take place within the high-temperature, high-pressure plasmas required for fusion energy. Areas of special strength include: the National Spherical Torus Experiment Upgrade (NSTX-U); the Lithium Tokamak Experiment (LTX); high-resolution techniques to measure plasma properties and processes at a wide range of space and time scales; powerful capabilities for plasma heating and current drive; capabilities for analysis of data from high-temperature plasmas used by experimental teams around the world; expertise in understanding, numerically modeling, and operating a wide range of magnetic confinement configurations; world-leading basic plasma experimental facilities such as the Magnetic Reconnection Experiment (MRX); and premier analytic theory capabilities that are internationally recognized as a continuing source of seminal ideas and mathematical foundations of plasma physics and fusion energy science.

Synergistic to these core capabilities, PPPL also possesses world-leading computational capabilities to accelerate the understanding of the physics of high temperature and burning plasmas (e.g., ITER) and discover new approaches. This includes codes for modeling small-scale plasma turbulence and associated plasma transport, nonlinear extended magnetohydrodynamics of larger scale plasma equilibria and motions, and wave-plasma interactions with plasma heating and the fusion-product induced instabilities possibly present in ITER. PPPL is developing advanced algorithms to enable efficient utilization of DOE-SC’s leadership-class computing facilities for fusion research including its new exascale computing initiatives. This allows us to validate physics-based predictive models against existing experiments, to investigate innovations to successfully development fusion energy, and use the integrated models to guide future ITER operations and experiments.

PPPL offers significant expertise and capabilities in advancing the understanding of the interaction of plasmas with materials. PPPL with Princeton University’s Engineering Department has established two surface analysis laboratories to study fusion-relevant material issues. PPPL established a nano-laboratory to study the plasma synthesis of nanomaterials of different types and compositions. PPPL also offers theoretical, computational, and laboratory capabilities in the realm of plasma astrophysics in areas such as plasma reconnection, the magneto-rotational instability, space weather, and high energy density plasma.

Approximately 116 FTE staff, including 22 postdoctoral fellows support this core capability. This core competency is the foundation for the Laboratory.

2. Large Scale User Facilities/Advanced Instrumentation

PPPL has extensive capabilities in: plasma measurement, heating, and current drive system design and construction; safe and environmentally benign facility operation including the use of tritium fuel; and specialized fusion confinement facility design and construction. These strengths together with an enormously capable research complex for fusion research (shielded test cells, high-current power supplies, extensive cryogenic facilities, and high-speed broadband network) support the operation of NSTX-U, aid the development and testing of components for ITER, and enable collaborations on major national and international fusion research facilities. PPPL is a partner with Oak Ridge National Laboratory (ORNL) and Savannah River National Laboratory in the U.S. ITER fabrication project and manages the U.S. role in ITER diagnostics and the ITER steady state electric network. These capabilities provide a flexible, capable platform for next-step U. S. fusion research facilities.

PPPL is internationally recognized as a pioneer in the development and implementation of fusion plasma diagnostics. It has provided diagnostics as well as the supporting expertise to many fusion programs around the world, often in collaboration with other U.S. institutions. PPPL’s seminal contributions have been particularly strong in techniques to measure in detail the profile of the plasma parameters (density, temperature, current density, and rotation), fluctuation diagnostics to measure the underlying
instabilities and turbulence responsible for plasma transport, and measurements of both the confined and lost alpha-particles produced by fusion reactions. PPPL has a long-standing, active collaboration program providing diagnostics to fusion programs around the world (JET, JT-60U, LHD, Wendelstein 7-X, Alcator C-Mod, DIII-D, EAST, and KSTAR).

The recent technical failures on NSTX-U underscore PPPL’s need to strengthen the Laboratory’s core capabilities. Several actions have been taken. A major reorganization of the top leadership of the Laboratory has taken place including the strategic acquisition of new senior experts in executive laboratory management, engineering management, project management, laboratory operations, and facility and infrastructure management. The NSTX-U project was reorganized under a Project Director with extensive management and technical experience with similar, challenging fusion energy research projects. A search is underway for a new Laboratory Director with demonstrated skills and experience whose contributions will be crucial to the transformation of PPPL. Comprehensive reviews relying on and benefitting from extensive expertise from across the DOE complex and international experts identified the root causes of the technical and operational failures in the lack of a framework for the application of the graded approach, the lack of ownership of components and the lack of distinction between project roles and compliance roles. Within an institutional corrective action plan, actions have been planned to provide, on a time scale consistent with the NSTX-U Recovery schedule, a framework for implementation of the graded approach, consistent with the resources available within the Laboratory. Roles have been defined in new role, responsibility, accountability and authority (R2A2s) documents to provide clear component ownership and distinct project roles and governance roles. New governance roles have been created: Chief Engineer and Technical Authorities. New procedures will define the requirements for the depth of the engineering rigor based on the level of risk determined for each component and will reflect the new ownership and governance roles. The release of the new procedures is staged and timed to support the NSTX-U Recovery schedule. At each stage, training will be provided to the relevant staff. Monitoring will be implemented to assess how the new roles and procedures support the operational discipline required to achieve the vision and missions described here. NSTX-U is discussed in more detail in Section 4.1.

Approximately 105 FTE staff support this core capability. This core capability is primarily supported by the Fusion Energy Sciences program. Recruitment and hiring in key areas such as mechanical engineering and systems integration are being ramped up to meet the need to enhance the Laboratory’s strengths while responding to the urgent need to respond to succession planning and attrition issues.

3. Mechanical Design and Engineering

PPPL is a fusion energy sciences leader in the confinement of a high-temperature plasma using magnetic fields. It offers demonstrated expertise in the design, analysis, and fabrication of large toroidal magnets, vacuum systems and in-vessel components capable of withstanding the harsh operating conditions such as very high heat fluxes, large electromagnetic forces, radiation fields, etc. These engineering capabilities span a wide range of disciplines and are well integrated with other capabilities at the Laboratory including plasma physics and electrical engineering. PPPL’s design engineers benefit from the challenges of designing and fabricating state of the art components for experiments under construction such as ITER; from the exposure to a wide range of technological advancements via collaboration within and outside the U.S.; and from the experience maintaining, modifying and operating on-site fusion experiments, such as, NSTX-U.

PPPL is performing the engineering and port integration of ITER diagnostics. The scope covers the design of equatorial and upper diagnostic port plugs, taking into consideration the design of the port cell infrastructure, interspaces and support structures as well as auxiliary components like windows and services such as cables and feed-throughs. A highly qualified and experienced PPPL engineer is leading the U.S. ITER Project Office (USIPO) effort on the design of the ITER central solenoid at ORNL.
PPPL maintains a strong engineering collaboration with DIII-D. As well as having assigned a lead engineer to GA, the team at PPPL has designed and manufactured several systems for DIII-D, mostly additional heating: the launchers for electron cyclotron heating; neutral beam lines components such as calorimeters, pole shields and logic control system; and plasma edge control devices, most recently a dual powder dropper.

Collaborations with laboratories and projects outside the U.S. expose PPPL engineers to the requirements of next generation nuclear experiments and the complexity of superconducting devices. PPPL has provided trim coils and in-vessel components to Wendelstein 7-X (W7-X), a flowing lithium module to EAST, electron cyclotron launchers to KSTAR and diagnostics for many collaborative efforts including JET.

PPPL’s engineering analysis staff is continuously expanding their simulation capabilities which include coupled multi-physics analysis of nuclear shielding, breeding, and activation; heat transfer; fluid dynamics of flow in magnetic fields and with free surface effects; transient nonlinear magnetics; and structural mechanics including advanced materials models.

Approximately 60 FTE staff support this core capability.

4. Power Systems and Electrical Engineering

PPPL offers both the physical infrastructure and technical competencies for meeting the extraordinary power system demands intrinsic to fusion energy research machines. The installed capability at PPPL can provide peak powers of ~1000MW and transfer 4.5 GJ of stored energy to magnetic coil systems. This capability overlaps that needed to address issues of transmission grid efficiency, reliability, and integration of variable generation. The utility-scale power systems at PPPL include a 138kV grid interface, large rotating machines used for energy storage, a local 13.8kV AC distribution system, and complex AC/DC converter systems using various power electronics devices and topologies. Magnet systems designed by PPPL for use on its experimental devices include solenoidal and toroidal configurations operating at 10’s of kV, up to 150kA, with 1000’s of MJ of stored energy. Advanced digital control and protection systems on PPPL devices involve feedback loops derived from advanced plasma diagnostic sensors as well as power system voltages and currents. PPPL’s engineering staff has deep experience in the design, fabrication, and operation of the diagnostic, control, protection, electromagnetic, and power systems as cited above, including proficiency in related design and simulation tools. These core competencies are directly related to the development of new power systems and electrical engineering technologies for transmission grid modernization and renewables integration. In addition, the PPPL infrastructure could be utilized as a test bed for various advanced technologies such as energy storage, advanced reactive power compensation, and power flow control, etc. The PPPL competency and infrastructure as cited above exceed those at any other DOE laboratory and most if not all international laboratories.

PPPL has also played a key role in the design of the ITER power systems, specifying, purchasing, and delivering the components and sending them to the ITER site. These were among the first components delivered to the ITER site by any of the ITER members.

Approximately 22 FTE staff, support this core capability.

5. Systems Engineering and Integration

PPPL has the capability to produce whole-system design, fabrication, and operation of fusion, plasma, and large electromagnetic systems. Systems Engineering and Integration is applied at three levels of fusion research. First, systems studies are applied at the reactor studies/concept stage. Second, systems studies are used to prepare for and conduct major construction projects. Third, systems simulations are used to improve the understanding of plasma operation and to control and protect large experiments.
On the first aspect, conceptual reactor studies, the lab provides leadership and key expertise in multi-lab integrated design teams. PPPL has provided the integrated engineering and physics system design studies of future U.S. and international facilities and programs including, the ARIES studies, the current Fusion Nuclear Science Facility (FNSF) Study, K-DEMO (S. Korea), and CFETR (China). The second aspect, systems engineering, is undergoing review and restructuring following the recent failures at NSTX-U as described earlier. The third aspect, systems simulations, relies on PPPL personnel with the experience to provide the numerical modeling and optimization of systems with simultaneous physics and engineering simulations.

PPPL is a world leader in comprehensive tokamak simulations using TRANSP, which integrates many physics simulations and is being extended to include plasma control and power systems. PPPL has developed many-parameter, multi-physics advanced real-time control systems, to optimize system performance while maintaining protection of the equipment. The newest of these systems is the NSTX-U Digital Coil Protection System, which combines the electrical and power systems controls of NSTX-U with mechanical performance models to provide combined electro-mechanical protection. This system was a reliable and valuable operational constraint during initial operations of NSTX-U. Such a system has been suggested to ITER and is of increasing necessity for the higher value, higher consequence protection of next generation reactors.

Approximately 15 FTE staff, support this core capability.

Science Strategy for the Future

As an innovation and discovery leader in plasma and fusion science and engineering for the nation and the world, PPPL has organized initiatives within our two core missions:

1. Understand plasmas from the nano- to the astrophysical scale.
2. Enable fusion to power the U.S. and the world.

PPPL is focused on understanding the plasma phase of matter, its interaction with electromagnetic fields, and other particles and forms of matter. This understanding and its related technologies have a broad impact on many scientific fields and applications, including fusion energy sciences, astrophysics and space sciences, plasma-material interactions and processing, particle accelerators, and high energy density plasmas. All of these areas are targeted in our strategic plan and impacted through PPPL’s research. PPPL’s work on fusion energy science is focused on understanding how magnetic fields can confine and control hot reacting plasmas.

PPPL’s four initiatives are identified below. They provide the tools for key scientific breakthroughs, increase understanding of plasma in key areas, and enable application of the understanding to national challenges including practical fusion energy. The initiatives support DOE program missions, broaden support from other agencies, address needs identified in workshop reports, and align with broader DOE planning documents. The initiatives are being initiated or pursued by Laboratory-Directed Research and Development (LDRD) proposals, and the choice of proposal topics submitted to solicitations by DOE and other agencies. PPPL will pursue these initiatives with multidisciplinary teams with expertise including theory, modeling, experiments, diagnostics, and engineering. The initiatives leverage investments by DOE in PPPL capabilities, staff, and infrastructure, and will sustain and extend PPPL’s core capabilities. Achieving the full success of these initiatives will require sustained effort and investment.
Infrastructure

Overview of Site Facilities and Infrastructure

The Princeton Plasma Physics Laboratory (PPPL) is located on 90.7 acres within the 1,750-acre Princeton University Forrestal Campus. The campus is punctuated by dense woods, brooks, and nearby streams; almost 500 acres remain in their natural state to protect and enhance the character of the campus. Immediately beyond the 500 acres and within eight miles sits two major highways, US Route 1 and the New Jersey Turnpike. The Laboratory is conveniently located 3 miles north of Princeton University, 36 miles southwest of Newark Liberty International Airport, 56 miles northeast of Philadelphia International Airport, 48 miles southwest of New York City, and 183 miles northeast of Washington, DC.

The Laboratory has 500 full-time employees, 6 joint faculty, 22 postdoctoral researchers, 40 graduate students. In addition, there are ~350 visiting scientists. PPPL utilizes 766,181 gross square feet (GSF) of the Princeton University Forrestal Campus in 30 Government-owned buildings and 2 trailers located at PPPL (“C” and “D” Sites) including one offsite (pump house). There are currently no leased buildings or facilities and no plans to enter into any external lease agreements. There were no real estate transactions during FY2016 and none are currently planned. For the Infrastructure Operations Improvement (IOI) Project, PPPL rented temporary office trailers in August 2016, for a period of 18 months, to house the staff displaced by the project.

As listed in the Facility Information Management System (FIMS) FY2016 report, the total Replacement Plant Value (RPV) of all PPPL facilities and infrastructure was $661M. The Non-Programmatic RPV was $481M. Every PPPL building asset utilization rating is greater than 95%, which is defined as “Over Utilized” by the Laboratory Operations Board (LOB) criteria. In FY2016, PPPL reported $118M of deferred maintenance (DM) after completing our final phase of 100% assessments by the known DOE Lab vendor, VFA. During this time period, PPPL worked directly with the Deferred Maintenance Sub-Team of the Operations Improvement Committee - Inter-Laboratory Working Group (OIC-IWG). This inter-laboratory team discussion sparked the need to more closely align our DM measurement methodology. After considerable efforts to better align with DOE guidance and insights gained through the OIC-IWG, the Laboratory re-classified categories such as building code upgrades, finishes and furnishings, and future life cycle forecasts. Estimates for FY2016 deferred maintenance should have been reported as $5M. PPPL anticipates these changes to be reflected in the upcoming FY 2017 estimate of $27M for deferred maintenance. While the alignment calculations re-established the baseline for the Laboratory at a lower number than previously reported, the existing infrastructure needs and requirements have not been reduced. PPPL’s repair needs remain at levels in excess of $130M. These significant demands are represented in the Deferred Maintenance Projections shown below. The needs remain real, and the Laboratory’s methodology continues to improve the accuracy of reporting.
SC Infrastructure Data
Summary

<table>
<thead>
<tr>
<th>Total Building Assets</th>
<th>30</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Building Assets Assessed</td>
<td>30</td>
</tr>
<tr>
<td>Total Area Assessed*</td>
<td>766,181 GSF</td>
</tr>
<tr>
<td>Total Other Structured Facilities (OSF)</td>
<td>26</td>
</tr>
<tr>
<td>Total OSF Assessed*</td>
<td>24</td>
</tr>
<tr>
<td>Total Deferred Maintenance ($)</td>
<td>$27,000,000</td>
</tr>
</tbody>
</table>

* NSTX and TFTR experimental OSF assets and office trailers are not summarized as part of the infrastructure

| Core Capabilities: Plasma/Fusion and User Facilities/Advanced Instrumentation |
|---------------------------------|-----------------|-----------------|-----------------|
| Condition                        | Adequate | Substandard | Inadequate |
| Buildings                        | 8        | 11           | 11           |
| Utilization                      |          |              |              |
| Under Utilized (GSF)             |          |              |              |
| Not Utilized (GSF)               |          |              |              |
| Excess (GSF)                     |          |              |              |
| Repurpose / Reuse (GSF)          |          |              |              |
| 25,571                           | 0        | 0            | 108,882     |

<table>
<thead>
<tr>
<th>Other Structures (OSFs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Condition</td>
</tr>
<tr>
<td>OSFs</td>
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</table>

The majority of the buildings on the PPPL campus are between 31-40 years old and 51-60 years old (depicted in blue and dark orange in the building age distribution chart below). Subsequently, there are 11 buildings classified as inadequate, 11 as substandard, and 8 as adequate (depicted in the red, yellow and green in the building condition chart below).
Campus Strategy

The Laboratory has developed a 10-year Campus Plan to focus on repairing the required core buildings needed to enable world-leading science and support the science strategy articulated above; to support the growing population of critical users by increasing space for employees, collaborators, researchers, visitors, and students; and to assure safe, efficient, and effective research operations. Our goal is to present a compelling plan to justify the construction of a new sustainable building in the future to replace aging facilities with high levels of deferred maintenance, creating green space, and addressing infrastructure needs with targeted GPP projects. Specifically, the infrastructure objectives have been realigned to fully support the NSTX-U recovery and operations, to enable more international collaborations, and to provide modernized, flexible, and safe laboratory space for small to medium experiments. This strategic plan will provide space that facilitates the collaboration, encourage the exchange of ideas, and provides the space for growth of mission specific programs. The Plan addresses how real property assets will be used to support the objectives of the DOE Strategic Plan and guidance provided by the Office of Fusion Energy Science and the Department of Energy. Planning is developed in accordance with the Real Property Asset Management Order, DOE O430.1C and the DOE-SC objective of integrating land use, facilities and infrastructure acquisition, maintenance, recapitalization, safety and security, and disposition plans into a comprehensive site-wide management plan.

While the overall size of the PPPL site is adequate for current and anticipated future needs, the condition assessment identified many substandard and inadequate facilities and utility systems on the site (as summarized in the previous tables and figures above). Mission readiness questionnaires were completed to fully understand scientific and operational short-term and long-term needs. The number of PPPL employees and activity mix has been growing over the years, the number of onsite collaborators and researchers has grown modestly as well. Personnel are currently doubled, tripled (sometimes quadrupled) in office space, causing collaborators and consultants to utilize any available conference room space while at PPPL. Utilizing conference room space creates a further issue for those who are in need of an actual conference room. In summary, because the needs have grown over the years, there remains a need for expanded office and meeting space to accommodate them.

In addition, the Laboratory is currently going through a substantial housekeeping effort. The following has been accomplished as of July 2017:
● Excess property disposition is 194% of the average for the previous five fiscal years;
● Scrap metal disposition is 165% of FY2016 and ~315% of FY2015;
● Electronics recycling is 161% of FY2016 and ~342% of FY2015; and
● Waste generation is 126% of FY2016 and 117% of FY2015

This lab-wide cleanup has made the most significant impact on the RF, CS, COB, ESAT, C-MG buildings, as well as the IOI trailers where the Laboratory has emptied 31 out of the 76 trailers, to date. While the Laboratory has much more housekeeping to do, the effort accomplished, thus far, has freed up Laboratory space providing the Laboratory with more usable real estate appropriate for small and medium experiments and testing lab space consistent with the science strategy above.

The Laboratory has increased its collaboration with Princeton University over the past two years, specifically related to computing. Princeton University’s High-Performance Computing Research Center (HPCRC), a 47,000-square-foot sustainable building situated on Princeton’s Forrestal Campus, is the centerpiece of Princeton’s innovative plan that provides robust computing resources to all faculty members and researchers. The Laboratory is currently working with the University to create a plan to merge PPPL’s infrastructure, currently located in the Laboratory’s Computer Center’s 4,000 square feet, into the HPCRC. Relocating PPPL’s computing center infrastructure into this facility will provide long-term efficiencies of scale and capability for PPPL, and readily host expanding PPPL capability for exascale-architecture computing and high-speed data access to ITER, other experiments, and leadership-class computing facilities, as articulated in Section 4.1 and 4.2. Discussions with FES are required regarding cost, schedule, and implementation.

The Laboratory is working with Princeton University on a number of other collaboration efforts. These include utilizing the University’s:

● Level 3 multi-factor authentication solution
● Learning management system
● Maintenance management system
● Document management system
● Space management system
● Existing hardware and software licensing opportunities

All of these efforts will greatly increase collaboration and decrease Laboratory indirect costs. The University has been very receptive to these increased collaborative efforts.

The gaps between the mission needs and the current conditions of the Laboratory are the following:

● Failing HVAC infrastructure that provides critical needs to support safe, uninterrupted operational conditions for NSTX-U recovery, which require
  o HVAC instrumentation and control replacements
  o HVAC equipment replacements
  o Process and controls air compressor system optimization
  o Roof replacements

● Lack of adequate space and environment for existing employees, collaborators, researchers, students, and visitors (short-term) and additional space (long-term)
Preponderance of shared office spaces
- Lack of optimal infrastructure to accommodate shared offices (IT, HVAC, lighting, privacy)
- Inability to locate appropriately “clustered” collaborators with the scientific need
- Lack of modern/updated, experimental and test lab space with flexibility to accommodate the changing needs of modern research
- Limited ability to accommodate even modest changes in scientific program without significant lab modifications (small, old style labs, limited infrastructure space, limited additional capacity of systems)
- Inability to accommodate new laboratory needs due to aging and inadequate infrastructure. (HVAC, electrical, instrumentation/environmental controls, fire systems, piping)

The Laboratory’s FY2017 maintenance budget is approximately $6.2M, or 1.3% of the Non-Programmatic RPV. The Laboratory is currently working on a plan to increase annual funding for Actual Maintenance to move toward a minimum of 2% of non-programmatic RPV. As shown in the Integrated Facilities and Infrastructure (IFI) Crosscut table, the deferred maintenance trend is established at a 2 percent rate as directed by DOE’s 2017 IFI Crosscut guidance. The Laboratory’s proposed projects and investments through the various funding sources are expected to reduce the forecast escalation.

The SLI-funded Infrastructure Operations Improvement (IOI) project began in FY2015 (with CD-1 approval) and provides a large initial investment toward implementing the Campus Plan. This project was initiated to address infrastructure needs including enhancing under-utilized space; eliminating aging structures which should not be re-purposed; repurposing existing space for greater utility; refurbishing aged offices, administrative areas, and R&D space; and enhancing PPPL’s ability to attract and retain technical talent in support of the Scientific mission. This investment will address $6.3M of deferred maintenance through the demolition of Mod VI ($899K), renovation of the LSB Annex ($553K), and the repurposing of the C-Site Motor Generator (MG) space into a centrally located machine shop ($4,850K). The Laboratory successfully achieved CD-2 in January 2016, and CD-3 in October 2016. Part of this IOI project includes the removal of 75 storage trailers. The Laboratory is making good progress and has cleaned out 31 storage trailers to date. The project is currently on budget and on time with a July cost performance index (CPI) of 1.01 and schedule performance index (SPI) of 0.94. The project is scheduled for CD-4 approval of IOI completion in October 2019.

To prioritize the allocation of infrastructure funding, PPPL uses the Mission Readiness Process. In the Planned Investments table, found below, the infrastructure funding is shown as individual items. The Laboratory also uses the Capital Asset Management Process (CAMP) to rank both capital and operationally funded improvements based on their risk and the benefit they provide to the Laboratory mission. In addition, the Laboratory is utilizing a newer, less subjective tool through VFA Inc.

In response to feedback last year, the Laboratory is creating a dedicated Project Management Office (PMO). This office will have dedicated professionals to manage both construction and science mission projects. During the past year expectations for project managers and principle investigators have been institutionalized. More projects have been added to the project portfolio. Project management performance and project oversight has improved over the last 6-8 months.
Infrastructure Funding Needs

The Laboratory cross-cut proposal for 2017 - 2028 (shown later in this section) includes the following key areas: repair core D-Site buildings, renovate rooms for additional office space, renovate buildings for small/medium experimental and test labs, demolish buildings and build one new building, and remove remaining contaminated tritium systems. At this time, the Laboratory has three immediate and three long-term priority infrastructure needs.

Immediate Priority Infrastructure Funding Needs

The first immediate priority infrastructure need is to address the failing HVAC infrastructure (instrumentation and equipment) that addresses the critical needs to assure safe, uninterrupted operational conditions for NSTX-U recovery. Over the past few months, a number of NSTX-U Recovery Design, Verification and Validation Reviews (DVVRs) have taken place (see Section 4.1). The reviews identified a number of infrastructure issues that need to be addressed to support NSTX-U recovery and operations. The HVAC systems are critical to the infrastructure of multiple buildings and pose a serious risk to the scientific mission. It is important to note that the Laboratory has begun design on the HVAC Instrumentation Systems in D-Site through the approved GPP design directive. This design phase is expected to go through FY2018. Beginning in FY2020, we are requesting funding for the next phase, which includes construction of the instrumentation phase, the design and construction of the associated HVAC equipment upgrades, and the expansion to other D-Site facilities.

The second immediate priority infrastructure need is to provide adequate space and environment for existing employees, collaborators, researchers, students, and visitors (short-term swing space) and additional space (long-term). Completing the outfitting of the CS Office Suite in the COB building to accommodate additional office space will alleviate the Laboratory’s short-term space needs. Repurposing 2,200 square feet of underutilized shell space will provide an additional ~30 workstations. Furniture for this space will be repurposed from the workstations currently in the temporary office trailers housing the staff displaced by the IOI project. Completing the outfitting of this space is listed as a GPP request and includes the installation of electric, lighting, HVAC with temperature controls, fire protection, data, and networking.

The third immediate priority infrastructure need is to fully utilize the Engineering Wing, which is a necessity for the Laboratory’s short-term workspace needs. One quarter of the Engineering staff currently reside in the temporary trailers. Returning the Engineering Wing to a habitable space is a priority and will be done to create a modernized and revitalized work environment for the employees, as this space will remain utilized until the construction of a new building (request described below) is completed. Preparing the Engineering Wing space includes mold assessment and remediation, replacing the badly worn carpet, improving the lighting, and updating the data and networking. Furniture for this space will be repurposed from the cubicles that are in the temporary office trailers to house the staff displaced by the IOI project. The design phase to renovate this space is currently an approved GPP project.

Long-term Priority Infrastructure Funding Needs

The first long-term priority infrastructure need is to provide adequate space and environment for existing employees, collaborators, researchers, students, and visitors (short-term and long-term). The Laboratory currently has 11 buildings classified as inadequate, 11 buildings classified as substandard, 10 buildings that are 51-60 years old, 2 buildings that are 41-50 years old, and
13 buildings that are 31-40 years old. The Laboratory has determined that by demolishing six buildings/facilities and constructing one four-story structure in its place, there would be a savings of $60M in deferred maintenance over 10 years. In response to the 2014 Annual Lab Plan Feedback, PPPL adjusted the campus plan strategy to focus on the removal of obsolete buildings/facilities to reach a more cost effective long-term plan. This represents a decrease in the amount of “inadequate” buildings on campus from 40% in 2014 down to <5% with the construction of the proposed new building, the completion of the IOI project, and the demolition of the targeted high-deferred maintenance buildings. This strategy will decrease our footprint while increasing green space, accessibility, visibility, security and collaboration. The proposed buildings to demolish hold 161 offices (averaging 162 sq. ft./office) and include the following: Admin Wing/Cafeteria, Admin Building/Library/Computer Addition, Engineering Wing, L-Wing, Laboratory building, and the Theory Wing. The demolition and construction will occur in a phased approach to accommodate the first and second (detailed below) long-term priority infrastructure needs. The new four-story building would become the “one-stop shop” at PPPL with all of our needs in one building. The “Scientific Collaboration Center” would hold offices, collaboration space, seminar/conference space, the cafeteria, library, space for collaborators and researchers, and just-in-time (JIT) space for visitors. The building would provide office utilization closer to 110 sq. ft./office, on average, and construction would be similar to the LSB annex office space rehabilitation currently underway (the IOI project). Existing experimental facilities would be relocated as articulated above. PPPL’s core utility infrastructure is well positioned for the new construction. Recently, PPPL completed both a chilled water distribution and steam distribution upgrade project. Additionally, PPPL is targeted to complete an electrical power distribution upgrade by 2019. In reviewing the central utility plant capacity requirements to support the site and the proposed new construction, PPPL has proposed a boiler equipment upgrade project (current GPP request).

The second long-term priority infrastructure need is to provide modern/updated, safe, experimental and test lab space with flexibility to accommodate the changing needs of modern research. Renovation of the RF, CS, COB, and ESAT (cleaned out due to the housekeeping efforts) and fit-out of the C-MG building will accommodate new and existing small and medium size experiments, in accordance with the science strategy as well as the Campus Plan. Existing experiments, currently housed in the Lab Building and L-Wing, will be relocated into one of these five buildings. In order to meet our strategic mission goals (see Sections 4.2, 4.3, and 4.4), the Laboratory is in need of modern, general-purpose research space that can adapt and customize to the ever-changing mission needs. These utility laboratories will serve both the foreseeable, immediate mission needs while being adaptable to accommodate and appeal to future generations of researchers. Both the RF and ESAT buildings have large, underutilized spaces in buildings with significant infrastructure deficiencies. While the inclination may be to demolish and rebuild new structures, the site utility infrastructure is integrated extensively through both buildings and rerouting them would cause project costs to become prohibitive.

The RF building has prime real estate that is now vacant following the extensive site-wide housekeeping effort. By replacing failing utility infrastructure and renewing the building envelope, the Laboratory will be capable of reliably supporting an investment in modern research laboratories. Underutilized space on the first, second and third floors will be transformed into zoned, modular research spaces. The fourth floor will serve as the mechanical service space for the floors below. These extensive renovations will address $7 million in pending Deferred Maintenance.
Similarly, outfitting and repurposing the ESAT building will provide medium-bay space for research and maximize usage of an unused section of an existing building. Medium-bay space is limited at the Laboratory and can be used for numerous research efforts, including coil winding. These renovations will address $1.7 million in pending Deferred Maintenance.

The third long-term priority infrastructure need is to remove and safely dispose of all remaining tritium hardware. The tritium systems at D-Site date back to the 1980s and would require significant rehabilitation in order to utilize them in accordance with today’s standards if the Laboratory were to have a program requiring their utilization. The Laboratory will be submitting a Field Work Proposal (FWP), which will identify a plan and mission need along with the funding request to complete this project.
SLAC NATIONAL ACCELERATOR LABORATORY

Lab-at-a-Glance

Location: Menlo Park, CA
Type: Multi-program Laboratory
Contractor: Stanford University
Site Office: SLAC Site Office
Website: www.slac.standford.edu

Physical Assets:
- 426 acres and 148 buildings
- 1.68 million GSF in buildings
- Replacement Plant Value: $1.69B
- 0 GSF in Excess Facilities
- 0 GSF in Leased Facilities

Human Capital:
- 1,524 Full Time Equivalent Employees (FTEs)
- 56 Joint Faculty
- 205 Postdoctoral Researchers
- 208 Graduate Students
- 0 Undergraduate Students
- 2,789 Facility Users
- 35 Visiting Scientists

FY 2016 Costs by Funding Source ($M)

- BES $346.9
- HEP $78.0
- ASCR $0.5
- EERE $2.9
- NNSA $1.9
- Other SC $12.8
- Other DOE $0.6
- SPP $16.4
- NP $0.3
- BER $4.6
- FES $5.5
- Other DOE $0.6

Mission Overview

Founded in 1962 with a 2-mile-long electron linear accelerator (linac), SLAC National Accelerator Laboratory (SLAC) quickly became the world-leading laboratory for accelerator design and detector development and, importantly, for revolutionary discoveries in particle physics. The linac was soon followed by construction of electron-positron colliders and, significantly, by the Stanford Synchrotron Radiation Lightsource (SSRL) which, as an early synchrotron radiation source, pioneered pivotal X-ray studies in materials, chemistry, and biology. To date, four Nobel Prizes have been awarded for research done at SLAC.

In the mid-2000s, SLAC continued our pioneering work in accelerator development by proposing what was then the radical idea to use a portion of the 2-mile-long linac to build the world’s first short-wavelength X-ray Free Electron Laser (XFEL). The Linac Coherent Light Source (LCLS) was commissioned in 2009, producing ultrashort, ultrabright pulses of coherent X-rays that transformed X-ray science and prompted a worldwide rush to replicate the facility. Recent demonstrations of X-ray self-seeding techniques, among others, have further enhanced the unique capabilities of LCLS.

SLAC’s mission is to be the world-leading laboratory for X-ray and ultrafast science, based on our leadership in electron accelerator physics and our distinguished history in applications of X-ray science.
to materials, chemical, and biological sciences. X-ray science plays a primary role in elementary particle physics in areas of theory, simulation, instrumentation, high-repetition-rate, fast-readout-detector technology, and massive-scale data analytics.

SLAC hosts more than 4,000 international researchers each year at our facilities and in lab-hosted science programs. In addition to operating LCLS and SSRL, SLAC operates the Facility for Advanced Accelerator Experimental Tests (FACET) for research on next-generation accelerator concepts. The Laboratory leads the DOE effort toward the construction and operation of the Large Synoptic Survey Telescope (LSST) and actively participates in the A Toroidal LHC Apparatus (ATLAS) detector at the Large Hadron Collider (LHC) in two dark matter searches and in experiments probing the fundamental nature of the neutrino.

SLAC’s success depends on a robust partnership with Stanford University, which manages the Laboratory for the DOE. Stanford attracts and supports some of the world’s best and most innovative scientists. SLAC jointly operates three institutes and a research center with Stanford: the Kavli Institute for Particle Astro-physics and Cosmology (KIPAC); the Stanford Institute for Materials and Energy Sciences (SIMES); the Stanford PULSE Institute; and the SUNCAT Center for Interface Science and Catalysis.

**Core Capabilities**

To ensure strong cohesion across our portfolio, SLAC is focused primarily on securing our position as the world-leading laboratory for X-ray and ultrafast science. The Laboratory also pursues a vigorous program in particle physics and cosmology aligned with national priorities set out by the High Energy Physics (HEP) and Nuclear Physics (NP) communities. These additional scientific programs drive the further development of our instrumentation capabilities, which in turn are critical to achieving our X-ray and ultrafast science center goal. We envision a comprehensive experimental and theoretical program to explore the leading scientific problems of the day, such as the nature of the neutrino, exploring the unknown in the highest energy collisions, the nature of dark matter and dark energy, the nature of cosmic inflation. We will take advantage of the synergy in the underlying science, the common technologies and capabilities required for experiments in these areas, and of the strength of our science and technical leadership.

SLAC has six core capabilities – **Accelerator Science and Technology; Large-Scale User Facilities/Advanced Instrumentation; Condensed Matter Physics and Materials Science; Chemical and Molecular Science; Plasma and Fusion Energy Science; and Particle Physics** – which together define the Laboratory as the nation’s leading institution for accelerator science and technology devoted to X-ray production; for the broad and deep science enabled by these technologies; and for particle physics and astrophysics. SLAC strategic plans continue to leverage and develop world-leading capabilities in these six core areas, described in more detail below.

These capabilities build on expertise developed in our earliest days. Starting with our first mission in 1962 to construct and operate the original 2-mile-long linac, SLAC developed core competencies in the fields of accelerator science and technology; designing, engineering, commissioning, and operating large-scale instrumentation and one-of-a-kind detector systems; and developing innovative computing solutions for data management and analysis. These capabilities served as the foundation for creating and hosting a series of successful, accelerator-based experimental facilities that have enabled research at the forefront of science. As a result of our expertise across all these technical areas and our ability to attract the best and brightest, both among scientific staff and external scientific users, SLAC quickly established ourselves as the world leader in elementary particle physics research, becoming the home of many revolutionary discoveries in the field. A succession of electron-positron colliders (SPEAR, PEP, and PEP-II), along with the world’s first and only linear collider Stanford Linear Collider (SLC), followed the original linac and became the site of further seminal discoveries at the frontiers of particle physics. The
Stanford Synchrotron Radiation Lightsource (SSRL) was also established using the SPEAR storage ring as a pioneering example of using a synchrotron X-ray radiation source to study the structure and properties of materials, chemistry, and biology, thereby broadening the range of scientific discovery SLAC facilities can enable and initiating the Laboratory’s development into a multi-program laboratory.

In addition to this legacy of leading the world in the field of accelerator science, SLAC became a pioneer in a multitude of other areas at the forefront of modern science, such as facility development; cutting-edge instrumentation, electronics, and data acquisition; real-time data reduction techniques; and innovative computing solutions for data intensive analysis. All these are critical factors in enabling current scientific experiments, both for high-energy physics and for photon science. Today and in the future, we see the world-leading core capabilities continuing to serve as a foundation for innovative and transformational science at SLAC. These capabilities were the basis for the rapid turn-on of the world’s first hard X-ray Free Electron Laser (XFEL), the Linac Coherent Light Source (LCLS) at SLAC in 2009. The early production of science at LCLS demonstrated the impact of such a transformative X-ray tool for scientific discovery across a wide range of fields. SLAC has continued to evolve into a multi-purpose laboratory over the last decade, exploiting the opportunities offered by our world-class X-ray sources, the unique relationship with Stanford, and the location within Silicon Valley to grow core capabilities in materials science, chemical science, and plasma and fusion energy science.

1. Accelerator Science and Technology

Accelerators form the backbone of SLAC’s on-site experimental program. SLAC’s innovative ideas in accelerator research and design have created a series of extraordinary achievements, including research that led to four Nobel prizes. Today, SLAC remains the premier electron accelerator laboratory in the U.S. and one of the top accelerator laboratories internationally. Our world-leading research in accelerator science and technology continues to lead to innovations in accelerators at SLAC, in the Office of Science and internationally and is leading the way to new generations of particle acceleration technologies, including X-ray light sources, linear and circular colliders, and advanced technologies for the accelerators of tomorrow. In 2016, this research resulted in more than 50 high-impact journal publications, including eight articles in Nature and two in Reviews of Modern Physics. These technologies enable the development of bright, coherent X-ray light sources – both free-electron lasers and storage ring light sources – and in Ultrafast Electron Diffraction (UED) and Ultrafast Electron Microscopy (UEM), thereby strengthening SLAC’s core capabilities in materials science, chemical and molecular science, and plasma and fusion science. SLAC’s preeminence in accelerator design finds immediate use in the development of particle physics facilities worldwide, including the design of future particle colliders, both linear and circular, as well as applications of accelerators in various industrial, medical, and security-related fields. SLAC also maintains a renowned accelerator education program – one of only a few in the United States – run in conjunction with Stanford. With 18 graduate students presently enrolled, SLAC is helping train future leaders in the field. Five of the seven most recent awardees of the American Physical Society’s Outstanding Thesis Award in Beam Physics came from the SLAC program.

Accelerator Science and Technology at SLAC encompasses the following broad areas:

**FEL R&D:** LCLS is the most advanced operational hard XFEL in the world today. Its associated, highly successful R&D program brings new capabilities to the user community on a continuing basis, approximately twice a year. The R&D program has demonstrated both hard and soft X-ray self-seeding, two-color FEL beams; a wakefield de-chirper to precisely control X-ray properties, such as reduced pulse length, control of the FEL pulse bandwidth, and user-defined X-ray pulse tailoring; up to 99 percent circularly polarized X-ray beams; ultrafast diagnostics technology; and advanced undulator technology. These developments drive the discovery potential of LCLS and all its future upgrades.
The current upgrade – the LCLS-II project – uses high-repetition-rate superconducting accelerator technology. In contrast to the pulsed superconducting European XFEL, LCLS-II will operate in a highly stable, 1-megahertz (MHz), continuous-wave (CW) mode. Major advantages of the LCLS-II technology include: stable heat loads on all optical components and the experimental sample materials, significantly improved electron and photon beam stability and quality, evenly spaced pulses that allow more effective data collection and management from the detectors, and ultimately higher beam power, providing the capability to feed many more undulator sources with more electron pulses.

SLAC is developing future advanced FEL techniques, including precision synchronization between X-ray, laser, and radio frequency (RF) systems; circularly polarized undulators for LCLS-II; and manipulation of bandwidth and duration of pulses to enable new capabilities in spectroscopy and dynamics. The goal of the FEL R&D program is complete control of spectral and temporal X-ray properties. The program includes X-ray seeding developments for transform-limited pulses, generation and measurement of sub-fs X-ray pulses; generation of multiple colors and pulses; ultrafast techniques, diagnostics and optics; and technology development. In order to extend the spectral range of future LCLS-II upgrades to 20 keV and to improve high repetition-rate UED/UEM, SLAC launched a comprehensive electron injector R&D program, which includes a superconducting radio frequency (SRF) electron-gun development.

**Advanced acceleration and RF accelerator R&D:** SLAC plays an internationally unique role in the development of novel accelerating methods, including beam-driven plasma wakefield acceleration (PWFA) and laser-driven dielectric acceleration (DLA). These methods promise accelerating gradients of GeV per meter (in the case of DLA) to tens of GeV per meter (in the case of beam-driven PWFA), which would revolutionize the world of compact accelerators used for medicine, industry, light sources, and teraelectronvolt (TeV)-scale linear colliders. The Facility for Advanced Accelerator Experimental Tests (FACET) is the centerpiece of the PWFA program, having operated as a DOE user facility from April 2012 until April 2016. For SLAC to maintain our leadership in this increasingly competitive field, FACET-II – the follow-on facility to FACET – is under development. FACET-II will be the only facility in the world capable of providing 10 GeV electron and positron beams in support of accelerator science R&D, with primary focus on investigating key R&D challenges of PWFA-based e+e- colliders and fifth-generation light sources.

Particle acceleration using DLA is an advanced acceleration approach with a wide range of potential applications, such as compact, low-cost accelerators and X-ray sources. Over the past three years, SLAC and Stanford have collaborated to achieve great progress in this developing field, including the first demonstrations of on-chip acceleration at both relativistic and sub-relativistic particle energies. Encouraged by early successes, in 2016 the Gordon and Betty Moore Foundation awarded $13.5 million to the Accelerator on a Chip International Program (ACHIP), an international collaboration led by Stanford to develop a working prototype tabletop accelerator based on this approach. Joint SLAC – UCLA experiments achieved substantial progress toward one of the first major milestones for ACHIP with demonstration of record high-gradients up to 1GV/m.

SLAC has systematically investigated the limits on RF breakdown phenomena in high-vacuum metallic accelerating structures. We have embarked on a new program that uses RF structures in a novel way, extending beyond the traditional 11.4-gigahertz (GHz) X-band regime to THz frequencies. This program is accompanied by research on next-generation, compact and highly efficient RF-to-THz power sources. SLAC stewards a unique integrated capability in RF power source and accelerator technology tapped by federal agencies, industry, and labs around the world. This program is the only one within the DOE laboratory system that integrates capabilities for concept, design, prototype, and construction of these power sources.

**Accelerator test facilities:** SLAC’s four accelerator test facilities span a range of beam energies and capabilities that enable researchers to find a beam perfectly matched to their experimental needs.
addition to FACET, the test facilities include the low-energy *Accelerator Structure Test Area* (ASTA) facility, the medium-energy *Next Linear Collider Test Accelerator* (NLCTA), and the higher-energy *End Station Test Beam* (ESTB), providing unique electron beam capabilities for detector R&D. With more than 330 users in FY 2016 from more than 130 institutions, 44 percent of them students and postdocs, these facilities support next-generation acceleration development, as well as a wide range of experiments in materials science, THz generation, Compton-scattered photon sources, photocathode R&D, FEL seeding, high energy physics accelerator component and detector development, and general accelerator R&D. The UED/UEM facility is presently housed in ASTA and provides the most advanced nano-UED facility in the world, complementing the XFELs. As is the case with the novel RF technology program, these programs are relevant for both SLAC’s increasing strategic partnership project (SPP) activities and the DOE-HEP Accelerator Stewardship program.

**Ultrafast Electron Diffraction (UED):** SLAC has successfully realized the first milestone of the UED/UEM roadmap, with a 100-fs megaelectronvolt (MeV) UED instrument at ASTA in 2015. SLAC UED continues to make progress both in expanding our ultrafast science reach and in UED performance improvements. In the gas phase UED, we have successfully transitioned from proof-of-principle experiments to investigating the unknown dynamics in chemical interesting systems. (Significantly, we conducted experiments on seven molecules between August and December of 2016.) We have also developed single-shot UED capability, which we successfully deployed to study phonon softening and non-thermal melting in warm dense matter.

The next milestone for the UED/UEM program is the development of an ultrafast UED user facility to support a broad user community. No such facility exists anywhere in the world. To control the emergent phenomena in quantum materials and access specific excitations in solids, we are developing a laser-based THz pump. First light of the THz source is expected in June 2017. We intend to develop a smaller probe, with better temporal resolution and higher flux, to attract a much broader user community. We also propose a UED farm, consisting of three or more independent UED beamlines for studying gas/liquid phases and condensed matter, with applications in physics, materials science, and biosciences.

SLAC is developing a gun-based, SRF UED/UEM facility. The SCRF gun will enable the development of MHz UED, which will be complementary to LCLS-II. A SCRF-gun-based, single-shot ultrafast electron microscope could achieve atomic spatial resolution (0.3 nm) and sub-nanosecond temporal resolution. The proposed microscope will make it possible to capture irreversible processes in materials science and biology, such as direct imaging of biologically important conformational transitions of macromolecules and glass phase transitions in real time.

*Funding for this core capability comes from DOE-BES, DOE-HEP, SPP customers, and LDRD investments. The core capability supports the DOE Office of Science (DOE-SC) mission in scientific discovery and innovation (SC 2, 22, 23, 24, 25, 26).*

2. **Large-Scale User Facilities/Advanced Instrumentation**

SLAC currently operates two Office of Science user facilities (LCLS and SSRL), with a third one, FACET-II, expected to begin operation in 2020. The Laboratory also operates the joint DOE/NASA Fermi Large Area Telescope (LAT) mission, and it is a major partner in several particle physics and astrophysics (PPA) instrument projects.

**Linac Coherent Light Source:** With its 1,065 unique users and more than 2,500 user visits in FY 2016, LCLS has matured into a robust facility, serving users studying ultrafast chemical dynamics, catalysis, quantum materials and extreme materials, biochemistry, and fundamental atomic physics. We have paid particular attention to increasing the efficiency and rate of user access. As a result, last year saw a 50 percent increase in experiments, a 27-percent increase in users, and an 18 percent reduction in the
overall cost of experimental delivery, allowing greater investments in preparations for early science on LCLS-II. We scheduled more than 5,500 hours of beamtime, with a sustained high availability of approximately 95 percent along with the highest ever level of multiplexing, such that more than 6,500 beamline hours were delivered. In 2016, there were 195 publications associated with LCLS – the second-highest level to date – including 25 publications in high-impact journals.

The facility continues to develop innovative modes of operation, with the past 12 months seeing the successful commissioning of a dechirper with exquisite control over the electron phase space to allow fresh-slice lasing and a multitude of multi-pulse, multi-color options. LCLS also noticeably improved data quality for the Coherent X-ray Imaging (CXI) instrument, achieving its highest peak X-ray power (0.3 TW at 9.4 keV), with sustained operation at 0.2 TW in 15 fs. As already noted, these innovations rely on our world-leading accelerator science capability. We successfully commissioned a seventh X-ray instrument, Macromolecular Femtosecond Crystallography (MFX), in the summer of 2016 and it has already delivered a range of full-scale user experiments and Protein Crystal Screening (PCS) tests. Further enhancements to LCLS are currently underway, including new X-ray transport mirrors to increase throughput and beam quality; a new split and delay unit to meet a major gap in capability; methods to create sub-femtosecond pulses; and a transformation of the functionality of the X-ray Correlation Spectroscopy (XCS) instrument to meet long-standing user demand. The many exciting areas of scientific opportunity for LCLS and its upgrades, along with the activities in preparation for LCLS-II, are described in detail in Section 4.

**Stanford Synchrotron Radiation Lightsource:** Building on core competencies that also support LCLS, SSRL serves more than 1,600 unique users annually and produced 554 publications and nearly 100 Ph.D. dissertations in 2016. SPEAR performance continues to be excellent, providing high availability at high-current (500 mA) operation. Ongoing R&D is directed at reducing the SPEAR emittance and at improving time-resolved capabilities. The R&D strategy at SSRL takes advantage of the history of collaboration between SSRL and Stanford, the strong research programs in chemical and materials science at SLAC, and the synergy between SSRL and LCLS.

All these areas of emphasis are evident in the SSRL research strategy: construction of an advanced spectroscopy beamline with support from the Joint Center for Artificial Photosynthesis (JCAP); construction of a metrology beamline in support of DOE and National Nuclear Security Administration (NNSA) mission needs; construction of a microfocus macromolecular crystallography beamline funded by Stanford and The Scripps Research Institute; collaboration with SIMES to develop an angle-resolved photoemission beamline coupled to advanced materials growth capabilities; coordination of R&D programs between LCLS and SSRL in superconducting detector development; and development of high average power X-ray optics.

SSRL’s strategic plan, developed in parallel with LCLS strategic plans and scientific opportunities to maximize SLAC’s overall priority to continue as the world-leading laboratory for X-ray and ultrafast science, will enable scientific advancement in four major focus areas: (1) accelerating functional materials discovery and design through incisive characterization; (2) understanding catalytic function with atomic-scale precision; (3) identifying how constituent interactions generate emergent behavior in quantum materials; and (4) characterizing complex biomachinery and heterogeneous hierarchical natural systems. On this basis, we will establish X-ray emission spectroscopy and high-resolution, fluorescence-detected absorption spectroscopies in the hard, tender, and soft X-ray regimes as standard spectroscopic methods for chemical, biological, and environmental sciences. This development leverages collaborations with LCLS in detector development and shared X-ray emission spectrometer capabilities, as well as collaboration with the Theory Institute for X-ray Spectroscopies (TIMES), in the Materials Science Division at SLAC. LCLS, SSRL, and SIMES jointly established TIMES, with the goal of providing a powerful theoretical framework to guide progress toward successful experimental outcomes and build a community devoted to understanding the theory of non-equilibrium phenomena underlying
many LCLS activities. We will also develop and expand micro-focus macromolecular crystallography in collaboration with LCLS. This new micro-focus undulator beamline at SSRL and the MFX instrument at LCLS represent the complementary cornerstones of this effort, providing a user gateway that will maximize effective use of LCLS while providing next-generation storage-ring-based capabilities.

**Particle physics and astrophysics facilities and instruments:** Taking advantage of SLAC’s core strengths in data acquisition, electronics, computing, and detector construction and operation, SLAC has made strategic choices to lead or engage in a specific set of major particle physics and astrophysics projects. To date, SLAC led the upgrades to components of the A Toroidal LHC Apparatus (ATLAS) detector at the Large Hadron Collider (LHC) and is a key contributor to the exploitation of LHC physics involving its world-leading theory group. As discussed below, SLAC is also exploring high-impact contributions to the national neutrino program with the Deep Underground Neutrino Experiment (DUNE) and pursues liquid Xenon-based technology for future neutrinoless double beta decay experiments.

SLAC leads the design, development, construction, and operation of the state-of-the-art Fermi LAT, launched in June 2008 on the Fermi Gamma-ray Space Telescope (FGST), a major space observatory for the study of high-energy processes in the universe. Expanding into dark matter and dark energy searches, SLAC is applying the experience gained from this program to the wide-field Large Synoptic Survey Telescope (LSST) in northern Chile, leading the design of the camera. SLAC is also engaged in the construction of the next-generation experiments for direct detection of relic dark matter. We are the lead laboratory for the Super Cryogenic Dark Matter Search (SuperCDMS) project, a collaboration between DOE and the National Science Foundation (NSF), and provide major system contributions to the LUX-ZEPELIN (LZ) project. We anticipate having a major role in the eventual development of next-generation experiments for precision cosmology with Cosmic Microwave Background (CMB) studies. Each of the sophisticated instruments employed in these experiments presents a unique set of challenges. The experience gained in their construction, commissioning, and operation – whether in space, in underground laboratories, or on remote mountaintops – is key to the successful development of future large-scale instruments for HEP and photon science.

**Advanced instrumentation:** SLAC is an international leader in the development of advanced instrumentation and computational tools to serve the needs of our current and future X-ray and HEP experiments. Notably, SLAC has long-standing, significant expertise and capability in managing very large experimental datasets and we are actively developing strategies for data acquisition (DAQ) and data management for LCLS-II and for future opportunities with LSST, ATLAS, and DUNE. Integration of detector and control electronics, data systems, computational science, and algorithm development is critical to the success of these future flagship facilities and benefits greatly from strong ties to relevant departments at Stanford. Recent notable accomplishments include system design for high-bandwidth DAQ (custom sensors, application-specific integrated circuits for detectors, storage and distributed access for 100-petabyte-class data sets); characterization and control of micron-scale photon beams; and highly automated instrument control. Applications include integrated X-ray beamlines and instrumentation for photon science experiments, ultralow background experiments for direct dark matter detection, space-qualified electronic systems, and computational resources for automated and optimized data collection and analysis.

A significant interest exists in investing in new quantum technologies, both at the Office of Science – in Basic Energy Sciences (BES), High Energy Physics (HEP), and Advanced Scientific Computing Research (ASCR) – and through collaborations with Stanford. These collaborations can provide qualitative improvements that allow LCLS-II and SSRL to make precision measurements in many areas of condensed-phase chemistry and materials science. Among these are emergent properties of electrons in high-Tc superconductors, strongly correlated electron systems, and topological states of matter. To play a leading role in the quantum information revolution, SLAC and Stanford need to make investments in both software (quantum algorithms) and hardware (the first generation of useful quantum computers...
will probably be superconducting qubits), which will allow the quantum simulation of problems previously only addressed in approximation (e.g., quantum chemistry). The goal is to use quantum mechanics for measurements of unprecedented sensitivity. The quantum sensors and amplifiers are perfect candidates for precision measurements of phenomena such as dark matter, inflation, gravity, and X-ray spectroscopy. SLAC has strong capabilities in the required engineering and support technology, as well as a team of world leaders in the field of superconducting quantum sensors. The ideal tool set includes the Detector Microfabrication and Nano-X laboratories planned at the new Arrillaga Science Center (ASC, formerly the Photon Science Laboratory Building, PSLB) at SLAC. Such a flagship suite of capabilities would form the foundation for the development of detectors and essential superconducting readout components for LCLS-II, the Cosmic Microwave Background Stage IV (CMB-S4) experiment, and ultra-light dark matter searches. They would also provide a unique capability in advancing superconducting and quantum limited electronics devices broadly for the DOE complex.

Funding for this core capability primarily comes from DOE-BES and DOE-HEP. Other sources include Biological and Environmental Research (DOE-BER), Fusion Energy Sciences (DOE-FES), internal Laboratory Directed Research and Development (LDRD) investments and Strategic Partnership Projects (SPP) from the National Institutes of Health (NIH). SLAC’s efforts support the DOE-SC mission in scientific discovery and innovation (SC 2, 21, 22, 23, 24, 25, 26).

3. Condensed Matter Physics and Materials Science

The history of condensed matter physics and materials science at SLAC is tied strongly to the development of SSRL as one of the first synchrotron light sources to address electronic and structural properties of matter. Over the last decade, the Materials Science Division (now also called SIMES, Stanford Institute for Materials and Energy Sciences) has developed a particularly strong program in materials science that leverages SLAC’s X-ray facilities and complements them with world-class materials synthesis, characterization, theory, and design activities. These efforts often involve partnerships with faculty in photon science at SLAC, in several departments at Stanford, and with researchers in industry.

Our research program focuses on four areas – quantum materials, ultrafast science, bio-inspired materials, and energy storage materials – each of which addresses significant challenges in DOE’s missions in science, energy, and security. These areas reflect (1) our world-class strengths in research on novel superconductors, topological systems, and other materials, where emergent behavior stems from the complex interplay of many degrees of freedom; and (2) our strong focus on engineering novel collective properties through nano-assembly of bio-inspired materials, as well as through low dimensional materials and interfaces. Our principal investigators (PIs) have been recognized for their scientific leadership via Lawrence Awards, Buckley Prizes, Dirac Medals, and membership in the National Academies, among many accolades.

These research programs couple directly to current and future LCLS and SSRL science. For example, we are pursuing approaches that fully exploit the high average power of the coherent LCLS-II beam using the exquisite spectral and temporal resolution achievable with resonant inelastic X-ray scattering (RIXS) techniques. Scientists from SIMES have been engaged with LCLS to help realize the ultrafast materials science strategy and to use light sources to carry out some of the key scientific lines of inquiry identified in recent Basic Research Needs (BRN) workshop reports on materials. Techniques for combining X-ray diffraction at LCLS with photoemission monitoring of the electronic bands have been shown to provide an important advance in our understanding of superconductivity.

As we look ahead, materials science will continue to represent important scientific targets for SLAC’s X-ray facilities at SSRL and LCLS. With the advent of next-generation X-ray facilities, a golden age of scattering and spectroscopy is emerging with unprecedented opportunities for studies at nano-to-microscopic-length scales and femto-to-picosecond time scales. Adding to the capacity already in place
at LCLS’s soft X-ray end station has enabled pump-probe RIXS for the study of the time evolution of coupled order parameters. Our efforts are helping to set the science agenda for materials spectroscopy at LCLS-II and LCLS-II-HE, the proposed high-energy upgrade to LCLS-II. These capabilities are critical for deciphering how charge, spin, orbital, and lattice degrees of freedom interact to produce emergent phenomena and exotic states of matter, and how materials operate out of equilibrium. Advanced spectroscopic techniques will play a pivotal role in detailed explorations of the electronic, geometric, and excited state properties of crystals, surfaces, interfaces, and complex nanoscale assemblies of atoms and molecules, and how this physics evolves with temperature, pressure, electric and magnetic fields, or other externally controlled parameters. This exploration is not only of intrinsic scientific interest, but also key for designing new materials with properties tailored for energy and other technological applications, on which the economic well-being and the energy security of the nation will continue to depend well into the future.

Funding for this core capability comes from DOE-BES, with related support from Energy Efficiency and Renewable Energy (EERE) and Laboratory Directed Research and Development (LDRD) investments, and serves the DOE-SC mission in scientific discovery and innovation (SC 2, 21, 22, 23).

4. Chemical and Molecular Science

Research in chemical and molecular science forms a significant core capability for SLAC. The research program in this area focuses around two themes: fundamental understanding of chemical catalysis and research at the frontier of ultrafast chemical science. Both programs developed over the past decade and have already achieved broad recognition for their quality and innovation, as well as for their uniqueness both within the DOE system and within the broader American scientific enterprise. The core capability in ultrafast chemical science benefits extensively from the proximity to and expertise associated with LCLS. At the same time, the impact and success of LCLS has been greatly enhanced by the Laboratory’s ultrafast science research program, which has opened and is continuing to open new pathways for the use of LCLS and LCLS-II. The research program further benefits from strong interactions with Stanford, as facilitated through the joint SLAC-Stanford PULSE Institute for ultrafast science. In terms of its scope, depth and experimental capabilities, the SLAC ultrafast chemical science program is unique both within the DOE laboratory system and among American universities. Major investments in similar programs, coupled with new XFELs, are being made outside the United States, most notably in Europe in conjunction with FEL capabilities in Hamburg.

**Chemical catalysis:** Research into the fundamental aspects of chemical transformation through catalysis is both a major scientific frontier and a field of great importance for energy storage and management. As such, research in this area is being carried out under DOE support both within the university system and within the DOE laboratory complex. The SLAC program, however, differentiates itself through our world-leading use of theory to provide a quantitative and predictive understanding of key problems in catalysis under realistic reaction conditions. Major challenges where new catalysts are essential include artificial photosynthesis, chemical fuels, energy storage, and sustainable chemical processes. Over the last five years, SLAC has jointly developed a theoretical description of surface reactivity and heterogeneous catalysis, electrocatalysis, and photocatalysis.

Within this program of predictive fundamental theory for catalysis, we developed a complementary experimental component with expertise in catalyst synthesis, characterization, and testing, including the use of distinctive capabilities provided by SSRL and LCLS. Catalyst characterization at SSRL facilities is an integrated component in developing catalyst synthesis methods with atomic precision that are essential in catalyst design, and has been further strengthened by the hire of a senior staff member at SSRL with a stellar background in this area. Unlike traditional catalysis research programs practiced elsewhere, which tend to be mostly empirical in character, modeling and theoretical predictions play a central role in SLAC’s research program. Our approach to advance chemical catalysis is supported by strong...
involvement of Stanford faculty, bringing expertise in catalyst synthesis, characterization, and testing through the SUNCAT Center. SUNCAT has achieved international recognition at the highest level, as documented by influential publications and recognition of the research leaders. The experimental groups at Stanford collaborate with the SUNCAT theorists. In addition, the experimental facilities at SLAC, and especially SSRL, are important to many Stanford groups.

The SUNCAT program provides the fundamental basis for the SLAC involvement in JCAP, where SLAC integrates theory and experiment with the goals of developing a mechanistic understanding of electrochemical CO₂ reduction and devising new catalyst design criteria for this process. This effort relies on extensive use of the operando synchrotron facilities at SSRL. The JCAP activities at SLAC are closely linked to the JCAP activities at Caltech and at Lawrence Berkeley National Laboratory (LBNL), where complementary experiments and theory are being developed.

**Ultrafast chemical science:** The second focus area investigates fundamental aspects of chemical transformation and dynamics at atto- to picosecond time scales. By measuring and modeling change on these time scales, we are able to understand fundamental processes of electronic and nuclear motion at their very different time scales. The SLAC research program is strongly coupled to LCLS, which provides cutting-edge capabilities for femtosecond measurements using coherent X-ray radiation.

Experimental capabilities provided by LCLS are complemented by extensive laboratory sources, including high-harmonics, time-resolved electron scattering, and time-resolved ultraviolet and soft X-ray spectroscopy, that permit access to dynamics occurring down to femto- and even attosecond time scales. We are currently applying these methods to study of non-Born-Oppenheimer dynamics, strong-field laser-molecule interactions, solution phase dynamics, non-periodic X-ray imaging, nonlinear X-ray optics, and, most recently, time-resolved studies of reduced dimensional systems. The experimental efforts are coupled to a strong theory program on excited-state molecular dynamics, which is supported by advanced computational capabilities. Research efforts emphasize the development of new experimental and theoretical methodologies for nonlinear X-ray spectroscopy to allow researchers to take full advantage of the high brightness and repetition rate of LCLS-II.

Funding for this core capability comes from DOE-BES with support from LDRD investments, and serves the DOE-SC mission in scientific discovery and innovation (SC 2, 21, 22, 23).

5. Plasma and Fusion Energy Science

The SLAC program in plasma and fusion energy science explores the research enabled by the unique combination of high-power lasers and the LCLS X-ray laser beam, focusing on the characteristics of high-pressure and high-temperature plasmas. This capability marks the beginning of a new era of precision in high-energy-density science. LCLS X-rays characterize warm dense matter states with an accuracy that can support or refute competing theoretical models. We apply precision X-ray Thomson scattering, Bragg scattering, phase contrast imaging, and near forward scattering techniques to investigate plasmons, phase transitions to new materials, relativistic laser-matter interactions, and high strain-rate material responses. These studies provide critical experimental tests of physics models for matter in extreme conditions, which are important for the design of full-scale fusion experiments and provide an understanding of structural, transport, and radiation physics properties of fusion plasmas. Important new results include the discovery of species separation in shocks and precision conductivity measurements in warm dense matter.

We are also researching particle acceleration in plasmas with high-power short-pulse lasers, work that is done in collaboration with researchers at FACET who are exploring similar acceleration with electron-beam-driven plasmas. Our experiments can resolve the femtosecond time scales and sub-micrometer spatial scales needed to explore advanced physics regimes for ion acceleration, such as enhanced target normal-field acceleration or radiation pressure. This approach has been successfully applied in recent
experiments that have demonstrated high-energy protons with 80-MeV energy. In addition, we are exploring laser wakefield acceleration to produce GeV electron beams and associated betatron X-rays for ultrafast pump-probe studies. The direct interaction of high-power short-pulse lasers is especially important for the understanding of Weibel-mediated collision-less shocks and magnetized shocks that can lead to very high-particle energies relevant to the physics mechanisms for explaining the origin of cosmic rays.

These ultrafast pump-probe experiments are enabled by investments in technology programs such as the development of cryogenic targets for high-repetition-rate studies of liquid hydrogen, deuterium, and other important materials for fusion research. In addition, the program develops probe techniques unique to ultrafast studies with X-ray lasers or UED.

Our experimental efforts are coupled to a new theory program that uses advanced computational capabilities. DOE-FES and SLAC supported a well-integrated high energy density (HED) physics theory team, which works closely with our joint institutes, KIPAC and SIMES. These collaborations have already led to better designs for LCLS experiments. State-of-the-art, three-dimensional particle-in-cell models and density functional theory provide experimental designs and specific predictions for dominating physics processes and allow the development of reduced models for implementation in large-scale calculations for fusion experiments.

Internationally, there is significant investment in HED science facilities and programs linked to XFELs, with the most substantial programs based at the European XFEL and at SACLA in Japan, where a petawatt laser system is now being installed. SLAC’s leadership in HED science continues through recent DOE-FES investments in our laser systems, thanks to our ability to operate at much higher power-per-X-ray-pulse and with better X-ray phase space control. In FY 2017, first experiments in this area will access important new regimes of pressure for materials science, stretching from fundamental studies of electrides to the assessment of higher density ablative materials for inertial confinement fusion (ICF). Other results have demonstrated high proton energies, control of streaming instabilities, and paved the way towards new transformative compact accelerator concepts. Short-term investments in a high-repetition rate, high-power laser would be needed to fully explore this new regime. Ultimately, installation of a higher power (petawatt) laser coupled to LCLS would provide world-leading infrastructure by combining CW high-peak-power X-ray pulses with a very powerful laser beam. This would represent a unique scientific opportunity, something no other FEL/LASER facility in Europe, Asia or the U.S. can provide in a cost-competitive way. Such infrastructure would open up unprecedented materials irradiation and plasma physics opportunities.

In consultation with the user community, we are developing a detailed plan that optimizes the layout and laser drivers of the Matter in Extreme Conditions (MEC) instrument to keep our world leadership in this area. The proposed modifications of the Far Experimental Hall (FEH) for LCLS-II-HE provide opportunities for additional space suitable for a petawatt-class laser driver together with appropriate radiation shielding walls. We will further demonstrate the viability of the experimental concepts in complementary experiments at user facilities and assess the viability of a stand-alone laser facility to support this effort.

_Funding for this core capability comes from DOE-FES and LDRD investments, and serves the DOE-SC mission in scientific discovery and innovation (SC 2, 24)._
SLAC’s high-energy physics program are driven primarily by the pursuit of high-impact science questions in the field, as identified in close collaboration with our world-renowned theory effort, but also by ensuring that we can make unique contributions to the successful construction of the required facility through our world-leading instrumentation capabilities. This has currently led to an emphasis on Higgs and discovery physics; dark matter, dark energy and inflation physics; and neutrino physics.

Since its inception in 2002, the Kavli Institute for Particle Astrophysics and Cosmology (KIPAC), a joint SLAC-Stanford institute, has become a leading center for particle astrophysics and cosmology. KIPAC acts as an intellectual incubator for new science opportunities in particle astrophysics and the nexus for scientific exploitation of related new facilities, given its ability to bring together the ideas and experience of the particle physics and astrophysics science communities. The particle physics theory group and the KIPAC particle astrophysics theory effort together pursue a broad spectrum of pioneering theoretical research across all areas of fundamental physics: inflationary cosmology, computational quantum chromodynamics (QCD), dark matter, and supersymmetry.

Using the Higgs boson as a tool for discovery and exploring the unknown: The ATLAS experiment at the LHC is exploring TeV mass scales and beyond with prospects for elucidating the properties of the Higgs boson and discovering new particles and interactions, two of the P5 science drivers. Given SLAC’s comparable experience with BABAR/PEP-II operations, engaging in collaborations at the LHC is a natural extension that makes excellent use of our expertise in theory and experiment. SLAC makes a significant contribution to ATLAS in the pixel tracking system, the DAQ and trigger systems, jet physics simulations, and in detector operations, as well as in R&D leading to construction projects for the high-luminosity detector upgrade. All these capabilities were developed historically as part of the BABAR/ PEP-II and Fermi LAT programs and are immediately applicable to or further enhanced by many technical challenges at ATLAS and its high priority physics program. SLAC is well-positioned to assume a major role in the construction of the forward timing detector, as well as the silicon inner tracker, which are the most important detector subsystems included in the planned LHC phase 2 upgrades. We have the infrastructure, technical, and scientific expertise in several key areas, including 3D and CMOS pixels, strip detectors, and high-speed data transmission and readout. SLAC has proposed becoming the U.S. pixel stave assembly site, based on our precision mounting and optical survey capabilities. Other critical components for the upgrade are the trigger and DAQ systems. Our Reconfigurable Cluster Element (RCE) is a good candidate for the inner tracker readout, and our expertise in trigger development will be vital to the success of the physics program.

Pursuing the physics associated with neutrino mass: The nature of the neutrino and many of its fundamental properties remain a mystery to particle physics, with profound implications for cosmology. SLAC has a long history of developing the experimental techniques incorporated in the Enriched Xenon Observatory (EXO) for neutrinoless double-beta decay (NDBD), which will demonstrate whether the neutrino is its own anti-particle. SLAC and Stanford are currently leading the Enriched Xenon Observatory (EXO) NDBD demonstrator experiment, sited in the underground Waste Isolation Pilot Plant in New Mexico, which uses 200 kg of liquid xenon enriched with the $^{136}$Xe isotope (EXO-200). The future for this program resides with the next EXO (nEXO), a multi-ton-scale experiment that may be located at SNOLAB in Ontario, Canada. The Nuclear Science Advisory Committee (NSAC) identified a ton-scale NDBD experiment as the highest priority new experiment for the U.S. Nuclear Physics program, with nEXO being a lead candidate for this project. From EXO-200 and elsewhere, SLAC has extensive experience in the design, construction, and operation of noble-liquid Time Projection Chambers (TPCs) using ultra-low-background materials along with high-performance, low-noise, high-bandwidth cold electronics. Our effort in the accelerator-based, long-baseline neutrino oscillation and charge conjugation parity (CP) violation program has already impacted the DUNE detector design. Based on the critical expertise we provide in the area of trigger and DAQ systems, prototypes of DUNE and DUNE itself adopted the SLAC RCE system. SLAC plays a crucial role in the development of the liquid argon, TPC
automated reconstruction software, and in optimizing the detector for supernova neutrino science. These efforts are natural extensions of expertise we developed during the BABAR and Fermi LAT programs, and other past experiments. Together, scientific exploitation of nEXO and DUNE position SLAC to become a leading center for neutrino science.

**Identifying the new physics of dark matter:** Although extensive evidence exists that dark matter dominates the matter density of the universe, the nature of this matter remains unknown to modern particle physics. Various theories suggest a weakly interacting massive particle (WIMP) as the dark matter candidate, possessing weak-interaction-scale cross-sections with ordinary matter. WIMP detection could be accomplished by fielding ton-scale experiments in mines deep underground, where backgrounds associated with cosmic ray particles can be adequately shielded. The detection of relic dark matter at an underground experiment would be a crucial complement to efforts underway to create dark matter particles directly at the LHC and at future energy frontier accelerator facilities.

SLAC is uniquely positioned to address this cosmological mystery through two leading "Generation 2" experiments to search for WIMP dark matter. SuperCDMS will allow direct searches for relic dark matter candidates at unprecedented levels of sensitivity at low WIMP masses, while the complementary LZ liquid xenon experiment will provide the world’s best WIMP sensitivity at higher masses. Both have been selected as next-generation, direct dark matter search experiments, with SLAC playing a designated lead role in the SuperCDMS project at SNOLAB. SuperCDMS exercises our expertise in cryogenic germanium sensors and photolithographic fabrication techniques for such devices. LZ leverages our capabilities in large-scale, low-background TPCs, as does EXO. SLAC has optimized the design and production of large germanium sensors for SuperCDMS and is establishing cryogenic test facilities and TPC system test capabilities for noble liquid systems for LZ and, eventually, for nEXO and DUNE as well.

More recently, new ideas based on an ultralight dark matter candidate (hidden photon or axion) have emerged as another possible dark matter theory. Ultralight dark matter searches would open up new pathways for physics beyond the Standard Model, with enormous unexplored phase space in mass and coupling (6 orders of magnitude in coupling and 9 orders of magnitude in mass). These ideas are being pursued with the Heavy Photon Search (HPS) experiment at the Thomas Jefferson National Accelerator Facility and potentially with new DArk Sector Experiments at a purpose-built LCLS-II beamline (DASEL), without any impact on LCLS-II X-ray delivery.

In a related activity, the FGST, a space-based gamma-ray observatory, is transforming our understanding of the high-energy universe. FGST has recently provided insights into the origins of some cosmic rays and has conducted a wide variety of searches for dark matter. SLAC was the lead laboratory in the construction and integration of the LAT and plays a critical role supporting instrument operations. The collaboration with NASA on FGST electronics brought with it experience in the design and construction of large-scale, highly reliable electronic systems for space use, which will also serve us well in the design of such systems for DUNE, where instruments will be similarly inaccessible during operation. The LAT provides a complementary tool for dark matter searches by seeking to observe a gamma-ray signal from the annihilation of dark matter in space. No evidence of such a signal has been seen yet, but the limits place constraints on relic dark matter and its properties that are complementary to those from direct search experiments. This combination of tools and active theoretical research in particle physics and cosmology makes SLAC, KIPAC, and Stanford a scientific powerhouse for dark matter research.

**Understanding cosmic acceleration: dark energy and inflation:** The dark energy that appears to be driving the accelerated expansion of the universe poses fundamental challenges to our understanding of quantum field theory and gravity. The detailed properties of dark energy can be constrained through a variety of methods, all relying on deep optical and infrared surveys of major fractions of the sky. The LSST project will provide a definitive wide-field, ultradeep survey of galaxies for precision measurement...
of dark energy properties. SLAC is leading the development of the project’s 3.2-gigapixel digital camera system and houses a vibrant dark energy research community at KIPAC. The camera project role is based on our long-term expertise in complex silicon detector systems, electronics, cryogenics, DAQ, and integrated instrumentation systems. As the host laboratory, we are working closely with the LSST Dark Energy Science Collaboration (DESC) to achieve its important goals of measuring dark energy with high precision. In parallel, we are developing a camera commissioning and pre-operations plan, along with an LSST facility pre-operations and survey operations plan jointly with the Association of Universities for Research in Astronomy (AURA) and the LSST Corporation. The combination of close ties to the LSST camera and data management projects, the planned operations support for DESC and LSST, and a strategic investment in dark energy research will make SLAC a powerful center for this science in the 2020s.

In the areas of inflation and the early universe, which pose profound questions for modern cosmology, SLAC and Stanford supported research with the Background Imaging of Cosmic Extragalactic Polarization 2 (BICEP2) experiment. In a joint analysis with the Planck Observatory, BICEP2 has provided the most stringent limits on B-modes from gravitational waves in the early universe. The CMB carries the imprint of cosmology and the forces from the inflationary period of the Big Bang, which defined the large-scale structures of the present-day universe. Such observations are expected to constrain the nature of cosmic inflation. BICEP3, deployed at the South Pole last winter, is a new instrument with a two-fold improvement in sensitivity and 10-fold improvement in survey capability over its predecessor. SLAC is also involved with the upgrade to the South Pole Telescope (SPT-3G) and the Atacama Cosmology Telescope (ACT) in Chile and its future evolution (Advanced ACT), all of which offer exciting opportunities for discovery. The ultimate experiment in this field, CMB-S4, will build on this and other pathfinder experiments to provide definitive measurements of the universe’s first light with a broad science scope that includes neutrino mass, CMB lensing, and cluster cosmology. SLAC’s unique expertise in superconducting device design and fabrication, the large-scale integrated focal plane assembly from LSST, along with plans to build suitable microfabrication facilities to allow large-scale production of superconducting devices, underpin both our CMB-S4 plans and new detector systems for X-ray applications.

Funding for this core capability comes from DOE-HEP and DOE-NP, as well as SPP from the National Science Foundation (NSF) and NASA, and LDRD investments. SLAC’s efforts serve the DOE-SC mission in scientific discovery and innovation (SC 2, 21, 22, 23, 24, 25, 26, 29).

Science Strategy for the Future

SLAC’s evolution over the past decade into a multi-purpose laboratory has taken advantage of a major opportunity that differentiates us from our peers: our unique relationship with Stanford, which is fundamental part of the strategic plan the Laboratory completed in September 2014.

The plan outlines the four pillars of our vision for SLAC: (1) innovating and operating premier accelerator-based facilities; (2) identifying and pursuing new science enabled by our facilities and defining the future direction of our facilities; (3) performing discovery, use-inspired, and translational research in energy; and (4) defining and pursuing a frontier program in the physics of the universe. Our six core capabilities, described above, and our core competencies in accelerator science and technology, instrumentation, X-ray science and technology, optical laser systems, and computer science underpin these strategic directions and set the foundation for our future growth and expansion.

Based on our strategic plan, we have recently focused our investments on two broad areas: photon science programs enabled by our X-ray user facilities (SSRL and LCLS) and particle physics and particle astrophysics programs. The Laboratory’s highest priority goal is to be the world-leading center for X-ray
and ultrafast science. In support of this focus, we have identified four major strategic initiatives aimed at delivering on our vision and making SLAC:

- The world-leading center for X-ray and ultrafast science
- An integrated center for theory, simulation, and instrumentation to explore the physics of the universe
- A world-leading center for electron accelerator physics
- An innovator for massive-scale data analytics

This compelling vision for SLAC ensures that the Laboratory continues to attract the world’s best scientists, both as researchers and facility users, who will expand the frontiers of science and provide innovative new technologies.

SLAC’s unique relationship with Stanford is a critical factor in our ability to realize this vision, and sets us apart from other labs in the DOE complex in several ways:

- Our strong sponsorship from Stanford President Marc Tessier-Lavigne, Stanford Provost Persis Drell (who served as SLAC director from 2007 to 2012), and Stanford Vice President for SLAC William Madia.
- Our ability to leverage our Stanford ties to attract the very best people and programs, including nearly 30 joint and term faculty appointments and four joint research centers with operations on both campuses.
- Significant investment from the University – $100M over the past five years – has helped transform the SLAC campus, adding critical infrastructure such as the Arrillaga Science Center, Stanford Research Computing Facility, SSRL beamlines, and cryo-electron microscopy (cryo-EM) facilities and capabilities.
- Our operating contract, which is built on a strong DOE-Stanford-SLAC partnership and was recently transformed by the Revolutionary Working Group (RWG) model aimed at improving trust between parties and restoring responsibility and accountability to line management at the lowest practical level of the organization.

Along with our world-class facilities and technical and scientific staff, our close ties with Stanford offer a unique opportunity for the DOE to advance scientific discovery across the spectrum of grand challenges identified by the Office of Science.

Infrastructure

Overview of Site Facilities and Infrastructure

SLAC’s campus sits on 426 acres leased to the DOE by Stanford located in unincorporated San Mateo County on the San Francisco Peninsula within a larger tract of land owned by Stanford, as described in Section 2 above. Major utility systems include electricity, cooling and hot water, domestic water, storm sewer, sanitary sewer, gas, fire alarm, telephone, and compressed air. Primary 230 kilovolt (kV) power is provided by a 5.4-mile DOE-owned tap line. The SLAC site includes tunnels and other unique experimental facilities, the largest of which are the 2-mile-long Klystron Gallery and the underground tunnel that houses the linear accelerator. With 45 percent of our buildings greater than 40 years old and utility distribution systems greater than 45 years old, reliability and maintenance of utility infrastructure is a significant challenge.

SLAC does not have any new leases of 10,000 gross square feet (GSF) or more, and there are not any dispositions of DOE land through leasing, sale, or gift in FY 2017. The terms of the most recent lease agreement between Stanford and the DOE identify up to 25 acres of land on the SLAC campus that can
be returned to Stanford in three phases. The first phase includes 12.5 acres shown in Figure 2; however, Stanford has not identified a timeline for any phase.

Campus Strategy

The SLAC Campus Strategy for infrastructure is focused on enabling our strategic initiatives, reducing risk, improving infrastructure reliability, minimizing life cycle costs, and enhancing operational safety and efficiency. With support from DOE and Stanford, SLAC is managing infrastructure risk and ensuring a sustainable platform for current and future science missions while leveraging the unique opportunities that exist in Silicon Valley and with Stanford.

The paragraphs below illustrate how SLAC aligns infrastructure investments with our strategic initiatives; the process for identifying and prioritizing infrastructure investments; the resulting risks; and how investments mitigate risk while supporting SLAC’s ability to accomplish our mission.

Aligning Infrastructure Investments with Laboratory Strategic Initiatives

Ensuring investments are properly aligned is critical to SLAC accomplishing our mission and strategic initiatives. The SLAC Long-Range Vision planning document provides a framework to ensure SLAC’s capital improvements and maintenance investments are aligned with our interconnected initiatives:

- The world-leading center for X-ray and ultrafast science
- An integrated center for theory, simulation, and instrumentation to explore the physics of the universe
- A world-leading center for electron accelerator physics
- An innovator for massive-scale data analytics

The SLAC Long Range Vision identifies infrastructure investments necessary to achieve these initiatives and realize the campus vision. For example, the Vision for 2020 is illustrated in Figure 2 below. Figure 3 on the next page further illustrates the alignment of infrastructure investments with SLAC’s strategic initiatives.

Figure 2: SLAC Long-Range Vision for 2020
Identifying and Prioritizing Infrastructure Risks

SLAC’s risk identification and mitigation process includes assessments of utility systems and buildings using DOE’s Condition Assessment Information System (CAIS) database; a balanced, risk-based prioritization process; subject matter expert (SME) review; business case analysis; and senior management team (SMT) stakeholder review and guidance.

The balanced, risk-based prioritization considers four risk areas: (1) mission; (2) environment; (3) safety and health; and (4) cost and schedule. This process, based on DOE’s Capital Asset Management Program (CAMP), results in a project ranking that is aligned with the SLAC strategic initiatives. This ranking is superimposed with life-cycle cost and Return on Investment (ROI) calculations that guide the investment strategy. Stakeholders and SMEs then analyze the resulting data and develop an investment plan for review and approval by laboratory senior leadership.

The risk based prioritization process includes a value-centric (life cycle costs and ROI) to infrastructure system renewal. For example, instead of replacing complete systems or equipment, we are reviewing systems at the component level to determine minimum levels of renewal or replacement that are required to meet mission availability goals. We also use test data to identify components that indicate a high probability of failure; equipment that tests within industry standards is monitored and retested on a periodic basis. This new approach is challenging our engineers to be more creative in designing systems to meet minimum requirements while providing options for improving ROI, life cycle costs, and performance goals.
Through this risk process, we have identified infrastructure risks and developed a comprehensive
investment plan as shown in the Infrastructure Investment Table (Enclosure 6). We are leveraging multiple
funding sources including SLAC Institutional General Plant Projects (IGPP), DOE-SL, and Stanford in these
infrastructure investments. Incremental investments are being made each year using IGPP funds to
address the most critical issues. These infrastructure investments will mitigate risk while supporting
SLAC’s Strategic Initiatives.

Infrastrucure Risks

In applying the risk identification and prioritization process, SLAC’s highest infrastructure risks have been
identified as: (1) electrical, (2) chilled water, (3) computing, (4) support office space, (5) and
underground utilities. We have also identified opportunities for risk reduction and improving mission
support through opening up site access and constructing a campus waste facility.

- **Electrical:** Our highest infrastructure priority is to reduce operational risks by providing adequate
electrical capacity capable of meeting current and planned mission needs, and to correct
significant code and safety deficiencies and operational limitations.

- **Chilled water:** The next highest risk is the reliability and efficiency of our aging and inadequate
cooling water infrastructure. The central cooling water systems, 1701 and 1801, are a key part of
this system and are more than 50 years old.

- **Computing:** Changes in mission capability require additional computing capacity for data storage
and analysis. Existing computing systems are not adequate to support multi-program data
analysis, scientific computing, data storage, and high-speed networking needs. SLAC currently
does not have a single facility capable of providing this management of data in support of our
multiple science objectives.

- **Support space:** Growth in mission capability necessitates additional staff support space. For
example, completion of LCLSII drives the need for new support space near the LCLS research area.
Laboratory infrastructure renovations are needed for some of the original buildings constructed
at SLAC that have been in operation since 1963. These assets support DOE’s science mission in
HEP and BES as well as in other areas.

- **Underground utilities:** Protect science facilities by repairing and replacing critical underground
utilities.

- **Open site access:** An open, accessible campus improves cross-collaboration of science users,
guests, and staff.

- **Campus waste facility:** Reduce risk and improve best management practices by consolidation of
hazardous waste operations into one centralized facility

Risk Mitigation Through Infrastructure Investments: Completed and Ongoing

With continued support from DOE and Stanford, we are refining our planning, processes, data
assessments, and analysis to manage our infrastructure risk and ensure a sustainable platform for our
current and future science initiatives.

In FY 2016, we completed the following site-wide infrastructure projects: Site Security Upgrade phase 2,
B040 High-Power Laser (HPL) lab, B027 Smart Grid Lab, B730 heating, ventilation, and air conditioning
(HVAC) replacement, B024 office renovations, and several other critical electrical, mechanical and
plumbing repairs.

In FY 2017, a large fraction of investments has been allocated to support the future infrastructure needs
of LCLS-II. Our second largest investment was in a partnership with Stanford to establish a cryo-EM
laboratory in Building 006 to further research capabilities in support of biosciences.
Also in FY2017, DOE, through the SLI program, invested in the K-Substation project that addresses our highest infrastructure priority of providing adequate electrical systems for the linac sectors 0-10. This project addresses operational risks and increases mission capability by replacing 12.47 kV to 480V substations and underrated 480V motor control centers, and providing additional electrical capacity. The project, which will initially support the LCLS-II program, will be completed in summer 2017.

Stanford has been a critical partner in investing more than $100M in our Laboratory over the past ten years by supporting our infrastructure needs and strategic initiatives. Stanford has funded the PSLB/ASC shell, the Guest House, the Kavli Building, the Stanford Research Computing center (SRCC), the Arrillaga Recreational Center at SLAC (ARCAS), and the Starbucks kiosk. Stanford also contributed to removal of trailers, recycled steel, and concrete materials to reduce risk and improve site appearance.

The Arrillaga Science Center (ASC), a key project currently underway, will provide centralized laboratory space with the necessary performance capabilities to grow our existing photon science research program. Co-location of laboratory capabilities and researchers will enhance science collaboration, productivity, efficiency, and functionality, and enable expansion of our photon science program. Leveraging our world-class user light sources – LCLS and SSRL – as well as PULSE and SIMES, SLAC will be well-positioned to support the level of research of an internationally leading photon science laboratory. To verify that the laboratory and office spaces designed for the ASC fit-out are matched to SLAC’s strategic vision, the ASC project team worked directly with senior management and associate laboratory directors, principal investigators, and support staff. Through these many one-on-one and group collaboration meetings, we gathered the science requirements and respective laboratory processes through interviews, confirmation meetings, sketches, requirement analysis, and work flow diagrams to complete ASC’s construction plans and specifications. The Stanford-funded and constructed ASC shell was turned over to SLAC in December 2016. The SLI-funded ASC fit-out construction commenced in February 2017 and will enable occupancy in summer 2018. The status of the ASC is illustrated by the Figure 4 photos below.

![Figure 4: Arrillaga Science Center Exterior and Interior](image)

In addition to buildings such as ASC, the most recent phase of the security infrastructure upgrade project expanded general access to a larger percentage of the site, supporting our goals of encouraging collaboration across disciplines by improving ease of movement around the campus. Completion of the site and security access improvement project this past year opened up additional campus areas (approximately 50 acres), improved flow of incoming personnel from the Science and User Support Building (SUSB – B053) to LCLS user facilities and offices, provided access to ARCAS, added tiered security for science buildings, and created a new pedestrian walkway from the Stanford Guest House to LCLS.

The ability to successfully grow and open the campus for collaboration depends largely on completion of the next phases. This will involve further reductions of the Accelerator Area footprint. The result will allow for the southern arc of the PEP Ring Road areas to become General Access Areas, providing...
greater flexibility for the use of existing buildings and developable sites to support future mission growth. Additionally, the existing main gatehouse on Sand Hill Road and the entrance area need upgrading. The gatehouse was built in 1999 and has since become the central site hub of access control, alarm monitoring, and dispatching, and there is insufficient space, electricity, and IT infrastructure. Furthermore, the main gate sees approximately 2,000 vehicles per day and is poorly designed to efficiently and safely handle that amount of traffic. The final phase of the Security improvements would include rebuilding the gate house, and improving the civil and traffic engineering design of the entry for vehicle, bicycle, and pedestrian access and improving safety for the Security Officers as shown in Figure D below. Enclosure 6 shows the estimated cost of these efforts: (1) reconfiguration and modernization of the main entrance and Sand Hill Road Security gatehouse (est. $2.9M in FY 2018) and (2) automation of gates/access control of the Linac Road and Research Yard (est. $3.7M in FY 2020).

Figure 5: Site Security Map

Risk Mitigation through Infrastructure Investments Upcoming
The required capital investments that address the infrastructure gaps identified in section 6.2.3 Infrastructure Risks are summarized in the Infrastructure Investment Table in Enclosure 6. Investments in these essential infrastructure systems will further support our mission to mitigate risk by bringing inadequate and substandard infrastructure on a path to adequate condition, as shown in Figure 6 below. Figure 6 shows that substantial progress has been made since 2012, and, with planned investment, significant progress will be made over the next decade. Planned infrastructure investments will enable safe and reliable operation of the existing facilities, reduce operating costs, and directly support SLAC’s strategic initiatives.

More specifically, these investments will support our science initiatives and ensure LCLS, SSRL, LCLS-II, FACET-II, Interaction Region 2 (IR-2), the Computing Center, and detectors are mission ready by 2022.
In addition to infrastructure investments by SLAC and Stanford, the following investments are proposed for DOE’s SLI program:

- **Medium and Low Voltage Revitalization (MLVR), linac sectors 10-30**: Like the FY2017 K-Substation project, this project addresses our highest infrastructure priority of providing adequate electrical systems for the linac. It will mitigate risk by revitalizing K-substations, underrated equipment, and variable voltage substation breakers for the remaining portion of the linac, sectors 10 through 30.

- **Chilled Water System Revitalization (CWSR)** improves inadequate cooling water infrastructure that is critical to LCLS, LCSL-II, FACET-II, and SSRL. Improvements in the cooling water systems will increase reliability, provide higher cooling system efficiency, and reduce operating costs by replacing aging systems.

- **Multi-Program Data Analysis & Computing Center (MPDC)** focuses on upgrading the site-wide computing center for all SLAC’s scientific statistics evaluation and computing needs. Both users and support personnel for LCLS, FACET-II, and SSRL have extensive computing needs. We anticipate user volume to grow to twice the current numbers when LCLS-II achieves first light in 2020. Moreover, the massive data challenge of LCLS-II will also place enormous demands on local computing and data storage needs. See the section below on Computing Infrastructure for more details.

- **Support office spaces**: The expected large influx of users and staff requires additional scientific office support space and collaboration areas. Technicians and scientists in these buildings are advancing SLAC’s R&D in synchrotron radiation light sources, advanced acceleration and RF accelerators, advanced instrumentation, particle physics and astrophysics, and facilities and instruments, and they are essential for SLAC’s continued growth strategy. Support office spaces could also potentially house the UED user facility. There are two options for meeting this growth need:

  1) **X-ray Science Support Building (XSSB)** provides essential support space for both users and support staff located at the LCLS campus adjacent to B901. XSSB will satisfy most of the projected staffing increases of laboratory growth. If XSSB is not funded, the CBRP scope will have to be expanded and accompanied by a major staff move to accommodate the LCLS/LCLS-II support needs. This project is a FY20 and FY21 SLI request as noted below, with construction completed in FY22.
2) **Campus Building Renovation Project (CBRP)** provides needed office support space for our scientists, users, and administrative staff by renovating existing buildings on the Main Campus. CBRP, a requested SLI general plant projects (GPP) investment, reduces risk by providing updated and renovated facilities to further support our science effort. CBRP will satisfy most of the projected staffing increases of SLAC laboratory growth. The CBRP will also support required renovations for laboratory infrastructure for some of the original buildings constructed at SLAC that have been in operation since 1963. These assets support DOE’s science mission in both HEP and BES as well as in other areas.

- **Site security and access improvements** will open the entire campus for cross-collaboration of science as described elsewhere in this document.
- **Radioactive Waste Management Facility (RWMF)** will provide a facility that addresses the diversity of hazardous waste operations being conducted around the site. With the planned campus growth, consolidating hazardous waste operations will reduce risk and improve best management practices.

**Excess Assets and Materials Plan**

While none of SLAC’s currently identified excess assets have been found to present an uncontrolled safety or environmental risk, their continued presence does burden our mission due to cumulative maintenance cost and inefficient use of land space. This space would be better used for modern office and laboratory facilities, improved parking, etc. In FY 2016, we removed and salvaged eight trailers and 23 Sea-Train/Conex storage units; rubblized 1,300 cubic yards (CY) of concrete blocks for reuse as road base; and removed and salvaged 4,300 tons of excess steel structures and frames. Stanford funded some of this removal. Future plans include removal of 41 trailers, 80 Conex boxes, 2,000 CY concrete blocks, 13 tanks, and two excess steel structures. The annual Certified Unified Program Agency inspection of hazardous waste/materials resulted in no violations of hazardous waste/materials requirements.

As trailers and excess facilities were removed from inventory, occupants moved into renovated or new buildings, increasing building utilization. Building utilization also increased in FY 2016 by doubling up employees in offices and converting common areas to offices and open office areas. We reviewed buildings to analyze where new staff could be added at little or no renovation costs and only furniture and move costs. This process, based on Facilities Information Management System (FIMS) standards, reduced under-utilized facilities from 16 to 10 percent. In FY 2017, we plan to further study utilization of buildings and improve full utilization.

Our priority is to continue our long-term vision and goal of consolidating personnel and functions from trailers into buildings, improving facility utilization rates, and removing trailers and other temporary structures deemed as excess assets. The Research Support Building (RSB) and Infrastructure Modernization project included a renovated single-floor Operation Support Building (B028: 20,355 GSF), a two-floor Administrative and Engineering Building (B041: 44,997 GSF), and a new three-story Research Science Building (B052: 65,544 GSF). SUSB (B053: 62,125 GSF) is a new four-story building housing the campus auditorium, conferencing center, site cafeteria, and administrative offices, replacing the previously inadequate auditorium and cafeteria. When completed, ASC (B057: 105,000 GSF) will fit-out a new laboratory and office square facility to continue this utilization improvement goal. (Note: current SLI funding will fit-out the first and second floors of the three-story building.) These SLI investments allowed us to vacate and prepare for the removal of inadequate facilities and have allowed 77 percent of our staff to work in either new or recently renovated buildings. Figure 7 shows the asset utilization.
While the overall staff numbers did not increase significantly, we increased building utilization with little or no renovation costs with increased building occupancy. This maximized our utilization of most of our buildings; therefore, we need XSSB and CRBP to provide office support space for our projected scientific growth.

SLAC’s current inventory of excess assets is summarized in the following categories:

- **Trailers:** We have developed a demolition plan, to address removal of these temporary structures over the next seven years. Since 2001, SLAC has removed 22 buildings totaling 46,349 SF and 48 trailers totaling 46,899 SF.

  In FY 2016, we removed 18 trailers from real property, totaling 25,176 SF and demolished six trailers, totaling 8,037 SF. Two trailers, totaling 3,595 SF, were transferred to a public university (UC Davis). SLAC has 39 remaining trailers totaling approximately 37,835 SF. These trailers are either shut down, slated for removal, being used for storage, or still functioning as office and laboratory space. The collective annual operational costs are $109K and annual maintenance costs are $57K; however, once a trailer is closed, its annual costs drop to less than $1K/year. Four facilities are currently declared as excess and are awaiting demolition in FY 2017 representing 3,214 SF and $11K in annual carrying costs. The estimated cost of removing them is less than $140K.

- **Buildings:** SLAC has identified several buildings and interaction region (IR) halls as excess assets. Most of the structures are concrete structures that are partially underground, not in use, and do not cost more than $1K each per year to maintain. The halls’ high bay structure and proximity to research facilities allow for them to be repurposed, as was done in IR-2, to create clean room space in support of the LSST camera construction and LZ test operations. The IR halls are also being used as storage facilities for LCLS and LCLS-II.

- **Other structures and facilities:** Once the PEP and SLC operations ceased, much of the equipment and ancillary infrastructure remained in place: two collider arcs (tunnels), beam dumps, substations, and cooling systems. The collider arcs are shut down and are awaiting a decision from DOE Office of Environmental Management (EM) on funding and subsequent deactivation and decommissioning (D&D). In 2009, DOE-EM agreed to acknowledge the collider tunnels for demolition, under a memorandum entitled “Environmental Management Transfer Decisions for Office of Science Excess Facilities and Materials.” The collider arcs pose minimal safety risk since they are inaccessible to unauthorized personnel; and there are negligible annual carrying costs associated with maintaining the space. For these reasons, the vacant space is used to store irradiated equipment until funds are available for D&D.

  Equipment in the PEP ring tunnel and support buildings, as well as the old beam dumps, will remain in place until they are deactivated. We are reviewing repurposing these concrete buildings for storage and other uses.
• **Excess accelerator materials:** SLAC developed a material release program that was approved locally in 2010 and led to the development of a DOE technical standard (DOE-STD-6004-2016) that now enables all sites to perform similar recycling operations while addressing the concerns of the 2000 DOE metal moratorium and suspension policy. Metals recycling at SLAC has now yielded 4,300 tons as of March 2017 and recovered $2M in recycling revenue. During the long-range period through FY 2025, this program should recycle materials from more than 10,000 tons of legacy accelerator equipment that no longer supports our mission.

In FY 2016, SLAC initiated an equipment removal project from the linac Sectors 0–10 and an equipment reconfiguration project in the beam switch yard (BSY) to facilitate LCLS-II installation work. The equipment removal and decommissioning aspects of the first kilometer of the linac was completed safely, on-time, and under budget in Q1 of FY 2017. The BSY equipment reconfiguration will be completed in Q3 of FY 2017. Use of this plan and of the recycling technical standard is resulting in a cost avoidance of millions of dollars compared to the costs of disposing the material as waste under the original moratorium.

Since 2006, disposal of legacy wastes has been a long-term priority and we have disposed 2,897 CY of radioactive and mixed wastes, and 422 excess radioactive sealed sources. Work slated to occur through FY 2019 will include the disposal of waste generated by the decommissioning project and completion of the disposal of the remaining 300 radioactive sealed sources. Long-term plans include the potential for a new RWMF that would greatly improve efficiency and reduce risk. Operation of the higher-powered LCLS-II and future LCLS-II-HE systems will increase the generation of activated materials. A modern, centralized waste processing facility will also minimize future accumulation of materials and reduce environmental risks. Conceptual work and site selection on this facility began in FY 2016. The facility also includes a radiological calibration facility necessary to support instrument calibrations for LCLS-II operations.

**Replacement Plant Value and Deferred Maintenance**

**Maintenance and Repair as a percentage of Replacement Plant Value (RPV):** The FY 2016 maintenance investment index (MII) at SLAC was 1.17 percent, a substantial decrease from the 1.5 percent stated in the FY 2005 ALP. The decrease is due to a 3 percent drop in maintenance spending and a 21 percent increase in adjusted RPV. Current forecasts show MII at less than 2 percent each year through FY 2028. Looking at the entire period, the average MII rate from FY 2016 through FY 2022 is projected to be 1.17 percent. Through a comprehensive maintenance assessment in FY 2015, increased planning activities in FY 2016, and continual condition assessment updates, SLAC has made significant progress towards determining appropriate funding levels for maintenance activities. These activities have also helped target maintenance investments to maximize mission readiness. SLAC will continue to build upon these recent MII improvements with the goal of meeting or exceeding the less-than-2 percent target each year. Figure 8 below shows SLAC at 8% RPV factor.

**Deferred Maintenance:** In our FY 2016 ALP, SLAC discussed the modified deferred maintenance projection that resulted from the Laboratory Operations Board-driven assessment. A more comprehensive review, including the re-evaluation of failure consequence to the scientific mission, re-characterization of equipment condition rating, inclusion of greater numbers of assets, reduction of asset maintenance intervals, and inclusion of cost escalation, has continued following last year’s submission. This now updated review has resulted in an increase in SLAC’s deferred maintenance of
$28.4M in the FY 2016 ALP to the $75.2M in the current ALP for FY 2017. The deferred maintenance is forecasted to trend down from 2017 through 2021, based on SLI funding and infrastructure investment, as shown in the Integrated Facilities and Infrastructure (IFI) Crosscut, and will begin to trend up again after 2021. If the plan described in these pages is implemented as proposed, the projected FY 2028 deferred maintenance will be $61.9M.

As shown in the IFI Crosscut table, the deferred maintenance trend is established at a rate as directed by DOE’s 2017 IFI Crosscut Guidance answers. This trend is expected to improve with continued investments through multiple funding sources, including laboratory overhead, SLI funding, and GPP funded primarily from DOE-BES and DOE-HEP. The planned capital investments that reduce deferred maintenance are shown with an asterisk (*) on the Infrastructure Investment Table below.

Figure 8: Benchmarking RPV at National Labs
THOMAS JEFFERSON NATIONAL ACCELERATOR FACILITY

Lab-at-a-Glance

Location: Newport News, VA
Type: Single-program Laboratory
Contractor: Jefferson Science Associates, LLC
Site Office: Thomas Jefferson Site Office
Website: www.jlab.org

Physical Assets:
- 169 acres and 68 buildings
- 880,269 GSF in buildings
- Replacement Plant Value: $415M
- 0 GSF in Excess Facilities
- 83,542 GSF in Leased Facilities

Human Capital:
- 699 Full Time Equivalent Employees
- 26 Joint Faculty
- 28 Postdoctoral Researchers
- 39 Graduate Students
- 9 Undergraduate Students
- 1,530 Facility Users
- 1,368 Visiting Scientists

FY 2016 Costs by Funding Source ($M)

- FY 2016 Lab Operating Costs: $184.1 million
- FY 2016 DOE/NNSA Costs: $177.8 million
- FY 2016 SPP (Non-DOE/Non-DHS) Costs: $6.3 million
- FY 2016 SPP as % Total Lab Operating Costs: 3.4%
- FY 2016 DHS Costs: $0 million

Mission Overview

The Thomas Jefferson National Accelerator Facility (TJNAF), located in Newport News, Virginia, is a laboratory operated by Jefferson Science Associates, LLC for the Department of Energy’s (DOE) Office of Science (SC). The primary mission of the laboratory is to explore the fundamental nature of confined states of quarks and gluons, including the nucleons that comprise the mass of the visible universe. TJNAF also is a world-leader in the development of the superconducting radio-frequency (SRF) technology utilized for the Continuous Electron Beam Accelerator Facility (CEBAF). This technology is the basis for an increasing array of applications at TJNAF, other DOE labs, and in the international scientific community. The expertise developed in building and operating CEBAF and its experimental equipment has facilitated an upgrade that doubled the maximum beam energy (to 12 GeV (billion electron volts)) and provided a unique facility for nuclear physics research that will ensure continued world leadership in this field for several decades. LDTJNAF’s current core capabilities are: experimental, theoretical and computational Nuclear Physics; Accelerator Science and Technology; and Large Scale User Facilities/Advanced Instrumentation.

The Lab supports an international scientific user community of 1,530 researchers whose work has resulted in scientific data from 181 full and 13 partial experiments (including 3 full and 3 partial in the 12 GeV era), 398 Physics Letters and Physical Review Letters publications and 1,377 publications in other
refereed journals to-date at the end of FY 2016. Collectively, there have been more than 130,000 citations for work done at TJNAF.

Research at TJNAF and CEBAF also contributes to thesis research material for about one-third of all U.S. Ph.D.s awarded annually in Nuclear Physics (31 in FY 2016; 562 to-date; and 200 more in progress). The Lab’s outstanding science education programs for K-12 students, undergraduates and teachers build critical knowledge and skills in the physical sciences that are needed to solve many of the nation’s future challenges.

Core Capabilities

The following core capabilities distinguish TJNAF and provide a basis for effective teaming and partnering with other DOE laboratories, universities, and private sector partners in pursuit of the laboratory mission. These distinguishing core capabilities provide a window into the mission focus and unique contributions and strengths of TJNAF and its role within the Office of Science laboratory complex. Descriptions of these facilities can be found at the website noted in the Lab-at-a-Glance section of this Plan.

Each of the laboratory’s core capabilities involves a substantial combination of facilities and/or teams of people and/or equipment, has a unique and/or world-leading component, and serves DOE/DHS missions and national needs. Specifically, TJNAF’s three major core capabilities meeting these criteria are described below in detail:

1. **Nuclear Physics** (funded by DOE Office of Science (SC) – Nuclear Physics (NP))

   **Experimental Nuclear Physics**

   TJNAF is a unique world-leading user facility for studies of the structure of nuclear and hadronic matter using continuous beams of high-energy, polarized electrons. The completion of the 12 GeV Upgrade project enables many outstanding new scientific opportunities. The 2015 NSAC (Nuclear Science Advisory Committee) Long Range Plan clearly stated that its highest priority was to capitalize on this investment: “With the imminent completion of the CEBAF 12 GeV upgrade, its forefront program of using electrons to unfold the quark and gluon structure of hadrons and nuclei and to probe the Standard Model must be realized.”

   The Continuous Electron Beam Accelerator Facility (CEBAF) electron beam can be simultaneously delivered to the experimental halls at different energies. With the completion of the 12 GeV Upgrade the beam energy can be up to 12 GeV, converted to 9 GeV photons for experimental Hall D, and up to 11 GeV to halls A, B and C. Each experimental hall is instrumented with specialized experimental equipment designed to exploit the CEBAF beam. The detector and data acquisition capabilities at TJNAF, when coupled with the high-energy electron beams, provide the highest luminosity \(10^{39}/eN/cm^2/s\) capability in the world. The TJNAF staff designs, constructs, and operates the complete set of equipment to enable this world-class experimental nuclear physics program. With more than 1,500 users annually, of which roughly 2/3 are domestic, TJNAF supports one of the largest, if not the largest, nuclear physics user communities in the world.

   The CEBAF science program spans a broad range of topics in modern nuclear physics. Recent lattice QCD (Quantum Chromodynamics) calculations predict the existence of new exotic hybrid mesons that can be discovered with the new 12 GeV experiments and elucidate the nature of confinement. New phenomenological tools have been developed that produce multidimensional images of hadrons with great promise to reveal the dynamics of the key underlying degrees of freedom. A surprising connection between the role of nucleon-nucleon interactions and the quark structure of
many nucleon systems discovered at TJNAF earlier, needs to be understood. Development of measurements of exceptionally small parity-violating asymmetries with high precision has enabled major advances in hadronic structure, the structure of heavy nuclei (through measurement of the neutron distribution radius), and precision tests of the standard model of particle physics, including a measurement of the electron’s weak charge.

Full operations of the 12-GeV science program are slated for FY18. Accelerator operations have been established to send simultaneous beam to three Halls. The new Hall D has completed its engineering phase and has started its science program. Hall A has successfully completed two experiments already. Hall C has established successful science operations and is ready to start its science program. In Hall B, all detectors are operational but work remains ongoing in FY17 on one superconducting magnet to complete the 12-GeV Upgrade Project.

**Theoretical & Computational Nuclear Physics**

A comprehensive theoretical effort with leadership across nuclear physics is the mission of the TJNAF Theory Center. The Theory Center has successfully established a unique three-pronged scientific effort, pulling together the state-of-the art theoretical, phenomenological and computational approaches, including the effective field theory techniques, QCD global analyses, and non-perturbative lattice QCD calculations. The research of the Theory Center focuses on ab initio calculations of properties and excitations of nucleons and mesons, the properties of light nuclei the properties of the nucleon-nucleon interaction, and the internal landscape of hadrons in terms of the spin, momentum, and spatial distributions of their constituents. The research program at the Theory Center is an essential part of the national and international effort to understand the internal structure of hadronic matter, and to explore the nature of quark and gluon confinement, which are of the highest scientific priorities of US nuclear physics, as articulated in the NSAC 2015 Long-Range Plan, and are critically important for the success of the 12 GeV CEBAF (and future EIC) experimental physics program.

The synthesis of the latest technology with innovative theoretical tools is particularly notable in the area of High Performance Computing. TJNAF deploys cost-optimized computing for Lattice QCD calculations as a national facility for the U.S. lattice gauge theory community that complements DOE’s investment in leadership-class computing. Computational techniques in Lattice QCD now promise to provide insightful and quantitative predictions that can be meaningfully confronted with and elucidated by forthcoming experimental data. An increasingly important part of this lattice effort is the computation of hadronic scattering amplitudes, with emphasis on providing the decay couplings of well-established mesons as a benchmark for extension to hybrid states, where the decay couplings will aid the experimental searches planned for the 12 GeV CEBAF program.

One of the key components in support of the 12 GeV experimental program is the Theory Center’s Joint Physics Analysis Center (JPAC) working closely with the GlueX and CLAS12 Collaborations. JPAC is developing theoretical and phenomenological understanding of production and decays of hadron resonances, which helps bridge the analyses and interpretation of experimental data from TJNAF with the results of Lattice QCD calculations.

Another key aspect of the Theory Center is that almost all of its members work very closely with the experimental community, in particular, in support of the CEBAF program. In addition, about half of the Theory Center members are engaged in the community effort and its phenomenological studies to help develop the strong science case for a future Electron-Ion Collider (EIC). By combining expertise of experimentalists, theorists and computing specialists from around the world, the Theory Center aims to employ advanced computer data processing and state-of-the art theoretical
and phenomenological techniques and tools to realize new insights into Quantum Chromodynamics and hadronic and nuclear structure.

The Nuclear Physics Core Capability serves DOE Scientific Discovery and Innovation (SC) mission numbers 2, 4, 22, 24, 26, 27, 28, 30, 33, 34, 35 and 36 from “Enclosure 1: List of DOE/NNSA/DHS Missions.”

2. Accelerator Science and Technology (funded by DOE SC – Nuclear Physics, High Energy Physics)

TJNAF has world-leading capabilities in technologies required for superconducting linacs; notably:

i) Complete concept to delivery of superconducting electron and proton linacs and associated technologies
ii) State-of-the-art SRF fabrication and assembly capabilities
iii) Unrivaled design, commissioning and operations experience in large cryogenic plants
iv) World-leading polarized electron injector capabilities
v) Low-level RF and controls
vi) Accelerator and large-scale control systems.

These world-leading capabilities are evidenced by the production of more than 90 cryomodules produced and in continuous operation today. The ability to deliver large projects on time and on budget is evidenced by our involvement in major superconducting projects for SRF and cryogenics, including SNS, LCLS-II and FRIB.

In addition, TJNAF has pioneered Energy Recovery Linac (ERL) concepts and technologies and currently hold the record for recirculated beam power (1.6 MW), and has been a world leader in high-power free electron lasers.

TJNAF possesses world-leading capabilities in beam dynamics aspects of linear accelerators, energy-recovery linacs, free-electron lasers and colliders.

Advanced Electron Ion Collider (EIC) Design

The Accelerator Division, in partnership with the Physics Division and collaborators at other national laboratories, has been developing a design concept for a Jefferson Laboratory Electron Ion Collider (JLEIC). A pre-conceptual design report for JLEIC was published in 2012, to respond to the energy and luminosity requirements of the EIC physics White Paper. The JLEIC design team, composed of TJNAF personnel and strategic national and international collaborators, is now working towards a pre-Conceptual Design Report (pre-CDR) in 1 to 2 years with a CDR to follow in ~3-4 years. Completing design and R&D towards a conceptual design report consistent with the critical decision timeline for the EIC project and with the requirements for DOE order 413.3.

The Accelerator Science and Technology Core Capability serves DOE Scientific Discovery and Innovation mission numbers 25, 26, and 30 from “Enclosure 1: List of DOE/NNSA/DHS Missions.”

3. Large Scale User Facilities/Advanced Instrumentation

Experimental Nuclear Physics (funded by DOE SC – Nuclear Physics)

TJNAF is the world’s leading user facility for studies of the quark structure of matter using continuous beams of high-energy, polarized electrons. CEBAF is housed in a 7/8 mile racetrack and was built to deliver precise electron beams to three experimental End Stations or Halls. The electron
beam can be converted into a precise photon beam for delivery to a fourth experimental Hall D. Accelerator instrumentation is installed to deliver beams to all four Halls simultaneously.

CEBAF provides a set of unique experimental capabilities unmatched in the world:

- Highest energy electron probes of nuclear matter,
- Highest average current
- Highest polarization
- Ability to deliver a range of beam energies and currents to multiple experimental halls simultaneously
- Highest intensity tagged photon beam at 9 GeV for exotic meson searches.
- Unprecedented stability and control of beam properties under helicity reversal for high precision parity violation studies.

Hall D is dedicated to the operation of a hermetic large-acceptance detector for photon-beam experiments, known as GlueX. Hall A houses two high-resolution magnetic spectrometers of some 100 feet length and a plethora of auxiliary detector systems, including the large-acceptance Super BigBite Spectrometer. Hall B is home of the 12 GeV Upgrade of the CEBAF large-acceptance spectrometer (CLAS12) with multiple detector systems and some 100,000 readout channels. Hall C boasts two roughly 80-feet long high-momentum magnetic spectrometers that allow for precision scattering experiments, and has housed many unique large-installation experiments. Maintenance, operations and improvements of the accelerator beam enclosure and beam quality, and the cavernous experimental Halls and the multiple devices in them, are conducted by the TJNAF staff, to facilitate user experiments.

The 12 GeV CEBAF science program will also require construction of additional experimental equipment, such as the MOLLER apparatus to measure the weak charge of the electron and provide a fundamental precision test of the Standard Model. Also foreseen is a general-purpose apparatus such as SoLID, that will allow unprecedented 3D imaging of nucleons in momentum space in the valence quark region, a search to new physics in the 10-20 GeV range complementary to the LHC but unique to a lepto-phobic Z’ of 100-200 GeV, and access to the QCD conformal anomaly.

To enable the experimental program, TJNAF staff is a world leader in the development and operation of high-power cryogenic target systems, and highly-polarized gaseous and solid-state target systems, such as polarized \(^3\)He, H and D solid-state polarized target systems, and frozen-spin H and HD-Ice targets. Many of these targets have demonstrated world record performance. In addition, to facilitate a modern and efficient data acquisition system, TJNAF staff have designed and developed an ultra-fast fully pipelined electronics system, with components finding their way into other user facilities such as Brookhaven National Laboratory. This development of advanced instrumentation allows for spin-offs such as that described in the bio-medical applications below. TJNAF staff is at present envisioning how with foreseen trends in advanced scientific computing and ultra-fast electronics, we can define the next generation of data readout of large-scale advanced instrumentation, as e.g. relevant for the envisioned SoLID apparatus and a future Electron-Ion Collider.

Nuclear Physics Detector Technology (funded by DOE SC – Nuclear Physics)

Developing and implementing novel detector techniques for the next-generation of nuclear physics experiments supports the main mission of TJNAF. Such techniques allow the development of large-scale particle identification, high-rate tracking and electromagnetic calorimetry systems. Some examples are the Ring-Imaging Cherenkov (RICH) kaon identification detector under construction in collaboration with INFN/Italy, the high-rate Gas Electron Multiplier (GEM)-based tracking systems in collaboration with University of Virginia, and the lead-tungstate (PbWO\(_4\)) based calorimeter
development in collaboration with Orsay/France and Catholic University of America. TJNAF is also instrumental in exploring scintillator readout utilizing position sensitive detectors such as multi-anode and micro-channel plate photomultiplier tubes as well as silicon photomultipliers (with their first-time ever applicability in a large-scale experiment in GlueX). In collaboration with ANL, TJNAF works on the development of a large-area picosecond photon detector. This expertise has contributed to the technology transfer efforts of TJNAF, as described in Section V, such as commercial breast cancer-imaging systems, the development of a new hand-held camera based on silicon photomultipliers and used as an imaging aid to cancer surgeons during surgical procedures, the advance of a SPECT-CT system that has been used in brain studies on awake, unrestrained mice, and development of PhytoPET, a PET imaging methodology for plant biology research.

**CEBAF Operations (funded by DOE SC, Nuclear Physics)**

As mentioned above, CEBAF has been recently upgraded to provide an electron beam with energy up to 12 GeV, a factor three over the original 4 GeV CEBAF design. In addition to the increase in beam energy, the maximum number of simultaneous experiments that CEBAF can support has been increased from three to four. The four-laser injector upgrade that is being installed is the last of the capabilities required to execute the simultaneous four-hall operations required of the accelerator. With 418 installed SRF cavities, CEBAF operations represent a significant fraction of the world SRF operating cavity-hour data set. Some of the CEBAF SRF cavities have been operating for more than 20 years. The CEBAF data set and operational experience is a valued resource for new or existing SRF based accelerators.

TJNAF staff has developed a substantial ability to conceive and design large accelerator facilities, building upon 6 GeV CEBAF operations and augmented with the ongoing 12 GeV Upgrade. With the completion of the 12 GeV Upgrade, TJNAF will continue its role of the world’s premier experimental QCD facility. The ability to use the TJNAF LERF as an accelerator R&D test-bed for Energy Recovery Linacs, and techniques required to establish cooling of proton/ion beams, for example, provides a mutual beneficial cross-fertilization between the TJNAF LERF and Nuclear Physics. In addition, the possibility of utilizing LERF in isotope production applications has been evaluated, and a proposal submitted accordingly.

**Accelerator Technology (funded by DOE SC – Nuclear Physics, Basic Energy Sciences, High Energy Physics, DOD ONR, Commonwealth of Virginia, and Industry)**

As a result of the development, construction, and operation of CEBAF, TJNAF has developed world-leading expertise in superconducting RF linear accelerators, high intensity electron sources, beam dynamics and instrumentation, and other related technologies. These capabilities have been leveraged to develop new technologies relevant to other disciplines beyond nuclear physics as well as applications to areas of national security.

Using SRF technology based on CEBAF, TJNAF constructed and operated an advanced Free Electron Laser (FEL). The development of this machine enabled TJNAF to pioneer new Energy Recovery Linac (ERL) technology. In the ERL, the electron beam is re-cycled back through the accelerator out of phase with the accelerating field so the beam energy is returned to the SRF cavities. This power, which would normally be dumped, can represent 90% of the beam power in a high power linear accelerator. A number of other laboratories are adopting this technology, and ERL technology is likely to become an important contribution to sustainability initiatives at DOE labs. TJNAF is developing a new plan for the future use of this valuable asset. The Lab is using the term LERF (Low Energy Recirculator Facility) to refer to this facility to reflect a broad potential. DarkLight is the first experiment to be staged in LERF; construction was partially funded by an NSF MRI grant and the first engineering run took place in August 2016. Other possibilities under discussion include
characterization of materials using low energy positrons and R&D on production of medical isotopes using the (gamma, n) reaction. Overall, TJNAF is developing these plans in response to program needs and scientific community interest for future utilization of the facility, to maximize the benefit to the mission of the laboratory and of the nation.

TJNAF is also applying its accelerator technology to collaborate with four other national laboratories to realize the Linac Coherent Light Source II, at the Stanford Linear Accelerator Center (LCLS-II at SLAC). TJNAF is responsible for construction of half (2 GeV) of the superconducting accelerator as well as the two cryogenic refrigerators.

**SRF Accelerator Construction (funded by DOE SC, Nuclear Physics)**

TJNAF has developed and installed state-of-the-art infrastructure for the design, development, fabrication, chemical processing, and testing of superconducting RF cavities. This complete concept-to-delivery capability is among the best in the world. All of these capabilities have been essential to the development, deployment, commissioning and operation of the 12 GeV CEBAF Upgrade and continue to be essential to refurbish cryomodules from CEBAF which is critical to maintaining the gradient needed to support the Physics programs. The completion of TJNAF’s Technology and Engineering Development Facility (TEDF) Project, provided about 40,000 additional square feet of space. The SRF Facility will be used to assemble the cryomodules for the LCLS-II project. Construction of the production cryomodules has commenced and will continue into early FY19.

**Cryogenics (funded by DOE SC, Nuclear Physics)**

Over the last two decades, TJNAF has developed a unique capability in large scale cryogenic system design and operation that is an important resource for the US national laboratory complex. The TJNAF cryogenics group has been instrumental in the design of many construction projects requiring large scale cryogenics: (SLAC (LCLS-II), Michigan State University (FRIB), Oak Ridge National Lab (SNS), TJNAF (12 GeV Upgrade), and NASA) as well as improving the cryogenic efficiency of existing systems (Brookhaven National Laboratory). In the process, many inventions have been patented, and one has been licensed by Linde (one of two companies that build cryogenic systems) for worldwide applications on new and existing cryogenic plants. This work has also resulted in many Masters theses to ensure the continuity of this expertise in the coming decades.

TJNAF’s cryogenics group’s highly-skilled staff operates and improves the laboratory’s five operational refrigerators including three large 2K cryogenic plants. The two Central Helium Liquefiers operating at 2K utilize patented cryogenic cycles developed by TJNAF that increase efficiencies by up to 30% as compared to what has traditionally been available from industry. This represents the largest and longest running installation of this type of cold compressors affording the lab the opportunity to gain operational experience that can be applied to similar existing or future installations. Further, this extensive operational experience has allowed the group to develop controls technologies and techniques that permit year round, unattended operations that drastically decrease staffing needs required for operations of this magnitude. Stepwise improvements have been made on the mechanical systems, primarily the warm compressors, which significantly extend their lifetimes between major maintenance cycles and decrease input power needs. The combination of cycle and mechanical improvements has decreased the input power requirements for equivalent refrigeration at 2K by 1.4MW for CHL2 as compared to CHL1.

The group is presently responsible for designing, specifying, procuring and commissioning the two CHLs for LCLS-II, based on the successful CHL2 design for the 12 GeV Upgrade and designs developed for FRIB. The FRIB refrigerator installation is nearing completion along with TJNAF’s scope of work supporting the project.
Nationally, this group is a premier source of cryogenic engineering and design for large helium refrigerators, filling a void in commercially available services. TJNAF’s cryogenics group is consulted when project needs for a large helium refrigerator system arise (>2kW @ 4K or equivalent capacity) to ensure effective design results and highly efficient operation.

The Large Scale User Facilities/Advanced Instrumentation Core Capability serves DOE Scientific Discovery and Innovation mission numbers 24, 26 and 30 from Enclosure 1: List of DOE/DHS Missions.

Science Strategy for the Future

The TJNAF science strategy for the future has a strong foundation based on the advancement of the US nuclear physics program (as embodied in the 2015 NSAC Long Range Plan) and the support of Office of Science accelerator projects utilizing TJNAF’s expertise in Superconducting RF and cryogenics technologies.

With the imminent completion of its 12 GeV upgrade project, TJNAF is well positioned to continue its world leadership in hadronic nuclear physics. The upgraded CEBAF along with the enhancements in experimental equipment offer many opportunities for major advances in the understanding of the substructure of the nucleon, the fundamental theory of the strong force QCD, aspects of nuclear structure relevant to neutron star physics, and the (lack of?) completeness of the standard model of particle physics. Full exploitation of the upgraded facility will require construction of new experimental equipment, and TJNAF has two proposed MIE projects (MOLLER and SoLID) that have received strong endorsement from the nuclear physics community.

The 2015 NSAC Long Range Plan (LRP) strongly supports the robust operation of CEBAF necessary to deliver the long-awaited science program: “With the imminent completion of the CEBAF 12 GeV Upgrade, its forefront program of using electrons to unfold the quark and gluon structure of hadrons and nuclei and to probe the Standard Model must be realized.” In addition, the LRP recommends “increasing investment in small-scale and mid-scale projects and initiatives” and we hope this can help realize the new MIE projects at TJNAF.

The 2015 NSAC LRP also recommends “high-energy high-luminosity polarized EIC as the highest priority for new facility construction following the completion of FRIB.” TJNAF is well positioned to provide the US nuclear physics community with a highly capable option for an EIC based on the cost-effective use of CEBAF as a source of highly polarized 12 GeV electrons. We continue to develop our novel figure eight collider design, known as JLEIC, and believe this represents an excellent opportunity for the US nuclear physics community and for the long-term future of TJNAF.

The 2015 NSAC LRP also identifies a theory initiative, “new investments in computational nuclear theory that exploit the U.S. leadership in high-performance computing”, that offers an opportunity to greatly advance progress in Lattice QCD calculations. TJNAF will strive to leverage its unique capabilities in high performance computing to address topics in QCD and other areas of computational science. In fact, TJNAF possesses key capabilities and competencies in accelerator science and in the application of the modern accelerator technologies. Continued development of these capabilities is one of the major initiatives integral to this strategic plan. In addition to providing world leading facilities and expertise to meet the identified needs of the nuclear physics research community, TJNAF has identified collaborative roles that it can play in the realization of facilities elsewhere associated with the Office of Science (e.g., Basic Energy Sciences and High Energy Physics) and other agencies. Most recently this has involved the Lab’s contributing to the FRIB and LCLS-II construction projects. It is anticipated that additional such contributions to other Office of Science projects, and also perhaps projects beyond SC, in the future. TJNAF is continuing to develop expertise in advanced computer science, visualization and data
management. TJNAF is a world leading center of Lattice QCD (LQCD) computing, and extending this competency to the experimental program complements the lab’s mission to maximize the scientific productivity of the nuclear physics community. TJNAF will continue to build on these developments with the goal of establishing this core capability in the near future.

Infrastructure

Overview of Site Facilities and Infrastructure

Thomas Jefferson National Accelerator Facility (TJNAF) is located on a 169 acre DOE-owned federal reservation within the City of Newport News in southeast Virginia. Adjacent to the federal reservation is the Virginia Associated Research Campus (VARC), a five acre parcel owned by the Commonwealth of Virginia and leased by SURA, the managing member of the JSA joint venture, which sub-leases five acres to DOE for use by TJNAF. Also adjacent to the federal reservation is an 11 acre parcel owned by the City of Newport News that contains the Applied Research Center (ARC) within which JSA leases additional office and lab space. Southeastern Universities Research Association (SURA) owns 37 acres adjacent to the TJNAF site where it operates a 42-room Residence Facility at no cost to DOE.

The TJNAF complex consists of 68 DOE-owned buildings comprising 880,269 SF of office, shop, technical, and storage space. JSA leases an additional 37,643 SF of office and shop space from the Commonwealth of Virginia in the VARC and 26,869 SF of office and lab space from the City of Newport News in the ARC. JSA leases 19,030 SF of storage space in two off site storage warehouses within 12 miles of TJNAF.

The TJNAF complex provides office and work space for 760 Federal Government and JSA contractor and subcontractor employees, a transient population of 1,530 users, and a total of 1,350 visiting scientists for periodic technical meetings and seminars hosted during a typical year. Facility space is well utilized with a current asset utilization index of 96.8%. Distribution of space by use is summarized below in Table 4.

<table>
<thead>
<tr>
<th>Type</th>
<th>Total Square Feet (Owned and Leased)</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Technical and Lab</td>
<td>263,163</td>
<td>38%</td>
</tr>
<tr>
<td>High Bay</td>
<td>151,175</td>
<td>22%</td>
</tr>
<tr>
<td>Storage</td>
<td>111,328</td>
<td>16%</td>
</tr>
<tr>
<td>Office</td>
<td>112,946</td>
<td>16%</td>
</tr>
<tr>
<td>Common</td>
<td>62,018</td>
<td>9%</td>
</tr>
</tbody>
</table>

The condition of TJNAF facilities is generally good (Table 5). Of the 73 DOE owned or leased buildings, 64 are rated adequate, eight substandard, and one inadequate. Of the four trailers, three were rated substandard and one inadequate. Of the 36 other structures and facilities (including OSF 3000 series assets) assessed, 33 were rated adequate and three substandard. A total of 10,495 SF of space is currently rated as underutilized and TJNAF plans to eliminate four trailers by the end of FY18. There are currently no excess facilities at the Lab and none are expected within the next ten years. There are 55 shipping containers representing 17,000 SF of storage space in use at TJNAF. TJNAF plans to remove 26 of these containers by the end of FY18.
Table 5: Facility Assessments and Excess Facilities

<table>
<thead>
<tr>
<th></th>
<th>Adequate</th>
<th>Substandard</th>
<th>Inadequate</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Count SF</td>
<td>Count SF</td>
<td>Count SF</td>
</tr>
<tr>
<td>Other Structures and Facilities (OSFs)</td>
<td>33 3</td>
<td>3</td>
<td>0</td>
</tr>
<tr>
<td>Mission Unique Facilities</td>
<td>32 328,650</td>
<td>11 266,601</td>
<td>2 8,314</td>
</tr>
<tr>
<td>Non-Mission Unique Facilities</td>
<td>32 360,246</td>
<td>11 266,601</td>
<td>2 8,314</td>
</tr>
<tr>
<td>Number and square footage of excess facilities</td>
<td>0 0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Square footage of underutilized space in non-excess facilities</td>
<td>4 10,495</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

TJNAF is entirely dependent on public utility service. JSA sources power from Dominion Virginia Power at an average rate of $0.055/kWh, water from The City of Newport News at an average rate of $5.08/KG, and disposes of waste water through the Hampton Roads Sanitary District at an average rate of $10.85/KG. Utility service meets mission requirements although occasional unplanned power commercial power outages periodically disrupt accelerator operation.

A current copy of the TJNAF Land Use Plan (Enclosure 3) can be found on the TJNAF Facilities Management website.

Campus Strategy

Infrastructure investments by the DOE and Commonwealth of Virginia added more than 199,000 SF of new or renovated facilities at TJNAF over the past 10 years to accommodate the CEBAF 12 GeV upgrade and large scale SPP projects such as LCLS-II. TJNAF has been a leader in adding high quality office and laboratory space on schedule and at the lowest cost of any DOE site. For example, TJNAF completed the 188,000 SF TEDF for $387/SF and will soon complete the 12,000 SF ESH&Q Building for $345/SF. Once constructed, TJNAF’s highly efficient facilities management program maintains these facilities for $11/SF (including utilities but excluding power for the accelerator operation). By comparison, commercial office space adjacent to TJNAF leases for $16-23/SF including utilities.

Despite these investments, critical infrastructure needed to effectively execute the TJNAF S&T mission remains unaddressed. Our campus strategy begins with the S&T mission described in the first four sections of this plan. Working with the CRO and the COO, the facilities planning team reviews the available infrastructure capabilities against the S&T plan and identifies current and projected gaps. We perform an analysis of alternatives (AOA) to identify the set of possible solutions to close the gaps between mission needs and infrastructure capability. The selection of solution and time phasing is driven by mission priority and constrained by the projected levels of GPP and SLI program funding.

Cryogenics Infrastructure

The Lab’s highest priority is Central Helium Liquefier (CHL) 1 Sub-atmospheric Cold Box Replacement (SLI-GPP) for Cold Box 1 in the Central Helium Liquefier (CHL) plant. In the last 24 months, two cold compressors within the cold box have failed resulting in early termination of the CEBAF science program. Cold compressor replacement parts are no longer available due to age of the equipment and TJNAF has repurposed all available spares. The first failed cold compressor was replaced by a spare from SNS while the original equipment manufacturer assessed the reparability of the original compressor, a task that is still continuing without resolution. The cause of the most recent failure is still undetermined but is similar to the first in that the rotating machinery in the compressor seized during spin down. Various options are being evaluated to restore the CHL to operational status in time for the Fall 2017
accelerator run but there is growing evidence the rotating machinery in CHL 1 is approaching end of life and further cold compressor failures may be expected in the coming year or two. Since the procurement and installation of a modern CHL 1 replacement will take between two and three years, immediate action is needed to maintain the planned accelerator operations schedule.

The End Station Refrigerator 2 (ESR2) (SLI-GPP) project is needed to provide additional cryogens to three of the four experimental halls to support the more aggressive 12 GeV experimental schedule and detector demand. The scope is to refurbish and install a 4K refrigerator from the Superconducting Super Collider (SSC) project with the associated distribution system, utilities, and controls. The existing End Station Refrigerator is 40+ years old and has insufficient capacity and reliability due to the lack of critical spare parts that are no longer manufactured or available.

Cryogenics Test Facility (CTF) Equipment Recapitalization (Lab GPP) is needed to continue upgrade of equipment critical to support testing for the cryomodule cavity components produced by the Superconducting Radio Frequency (SRF) Institute for Jefferson Lab, other Labs in the Office of Science complex, as well as SPP. The equipment is past its useful life and has been experiencing a higher fail rate. A new 4K cold box and controls were provided under the UIM project providing additional CTF 4K capacity and improved reliability. Additional investments are needed to increase 2K capacity and overhaul/replace aging equipment related to 2K operations. These investments are planned on a not to interfere basis for delivery of LCLS-II cryomodules in order to support anticipated future SRF projects for the DOE National Lab complex.

Office Space

CEBAF Center Renovation (SLI-GPP/Indirect) – The 1988 built structure has been rated as substandard. The mechanical system in this portion of the building has exceeded its service life and is exhibiting high and increasing failure rate. Replacement of major HVAC equipment is required in the near future. Replacement of the HVAC system will require vacating the portion of the building under renovation and removal and replacement of the ceilings. Lab staff and office equipment is currently overflowing into common areas such as corridors, storage rooms, and utility rooms creating egress issues and safety concerns. Reconfiguration of the affected spaces is needed to alleviate many of these conditions. Renovation will meet high performance building standards. The renovation will be executed one wing per year using GPP funds. The atrium/auditorium will be renovated in the fourth year using facility maintenance funds.

CEBAF Center Wing D (SLI-GPP) – CEBAF Center Wing D will be a 14,000 SF addition to CEBAF Center. The Lab is leasing 6,755 SF of office space in the Applied Research Center for the JSA Center for Advanced Studies of Accelerators (CASA) staff and it is necessary to co-locate CASA with Theory, Physics, and Accelerator Divisions in CEBAF. Further, this move will eliminate lease spaced that costs nearly twice the O&M cost of DOE owned facilities at TJNAF. This new addition will accommodate CASA as well as relieve overcrowding in the existing Wings A–C. Construction will meet high performance building standards and contribute to lower recurring utility cost.

High Bay Space

Physics Technical Support Building (Lab GPP) – Currently, technical staff and equipment supporting the operations for all four experimental halls are spread among several buildings on the campus and accelerator site. This new building will provide 14,000-16,000 SF of technical and high bay space for fabrication and will improve continuity and efficiency by consolidating these functions in closer proximity to the experimental halls. Additionally, the project resolves space shortages of Engineering Division technical and high bay fabrication space also currently distributed in multiple buildings. For example, Cryogenics Fabrication currently occupies temporary space in the ESR2 Building which is needed for the new ESR2 helium refrigerator plant.
**Experimental Equipment Lab Renovation** (SLI) - Renovation of the Experimental Equipment Lab building is needed to increase the functionality and utilization of the high bay space as well as to correct substandard mechanical systems, improve efficiency of the building envelope, and correct code deficiencies. The scope of the work will require vacating large portions of the building during the periods of construction. Functions will be temporarily relocated to the newly constructed on-site warehouse to minimize the impact on operations.

**Storage Space**

**Storage Building (Lab GPP)** – The Lab currently leases a 9,755 warehouse about 11.5 miles away from the site to store long term need materials and a 9,275 SF warehouse which is leased for LCLS-II. The Lab also has more than 55 shipping containers (totaling 17,000 SF) inefficiently being used for storage. This project would provide a 15,000 SF onsite storage building to replace the offsite warehouses and the shipping containers. The consolidation process for these materials will include validation of future material needs and elimination of unneeded material.

**Shipping and Receiving** (Lab GPP) – The existing shipping and receiving function is currently located within the Experimental Equipment Laboratory Building (EEL) among Physics technical areas. Relocation of the shipping and receiving function will make available additional technical and high bay space within the EEL Building to support experimental apparatus assembly and will improve campus continuity.

The storage, shipping and receiving, as well as the Facilities Operations Building will be constructed as one building in phases based on Lab annual GPP funding. The storage element will be the first phase of construction.

**Facilities Operations Building** (Lab GPP) The facilities maintenance shops are currently located in the Forestry Building (2,904 SF) constructed in 1970 which is leased from the Commonwealth of Virginia and is in substandard condition. Adjacent to this building is an unconditioned DOE owned building which is used to store material. Both buildings need to be replaced. The Facilities Operations Building will be constructed as an additional phase/addition to the Storage and Shipping & Receiving building.

**Road Improvement** (Lab GPP) Reconfiguration and improvements of Lab entrance roads to improve site coordination with adjacent land development.

**Anticipated Future (10 Year) Infrastructure Gaps**

Additional office space would be required to support additional staffing and scientific community users associated with major science program construction and operation. Space is available to construct a 70,000 SF wing addition on CEBAF Center for offices and meeting space.

The gaps can be closed using a combination of SLI, SLI-GPP, and NP-GPP funding totaling $90M. A majority of the above mentioned gaps can be closed over the next ten years, although using the prescribed funding profile through 2023 and then using $3M per escalated starting in 2024 only results in $81M in funding. These projects will eliminate more than $3.7M of deferred maintenance. Additional estimated funding of $2.0M is expected through a Utility Energy Services Contract to implement energy conservation measures. A well-funded GPP program for a lab the size of Jefferson Lab would be $3-4M per year.

The Lab’s Asset Condition Index is 0.99, a rating of excellent. The Lab has averaged 1.5% for maintenance and repair expenditures over the last 5 years. In spite of modest expenditures for maintenance and repair over the last five years (only 1.5% on average), deferred maintenance has decreased from $15.8M to $4.7M through SLI and GPP capital investments and the elimination of
temporary facilities. Over the next few years, however, deferred maintenance is expected to increase due to reduced spending as a result of the budget. Additional indirect funding of maintenance and repair is needed to increase total spending to about 1.8% to manage this expected deferred maintenance increase.

Electrical, mechanical, and fire protection preventative maintenance costs have decreased through the conversion from contract to in-house resources. Enclosure 2 is the Integrated Facilities and Infrastructure Crosscut Data Table showing planned Lab maintenance and deferred maintenance projections. FY17 is the last year for repayment of the 2002 Bonneville Power Administration financed energy project making the repayment funds available to allocate for repair and maintenance.

The Campus Land Use Plan is shown as Enclosure 3. Enclosure 2 shows the investments needed to implement this Campus Plan. The plan consists of a mix of SLI, infrastructure crosscut, NP-GPP, and alternative financing. NP-GPP funding levels shown were based on the annual NP budget guidance. It is not anticipated there will be any inadequate facilities at the end of the period.
Lab-at-a-Glance

**Location:** Idaho Falls, ID  
**Type:** Multiprogram Laboratory  
**Contractor:** Battelle Energy Alliance  
**Site Office:** Idaho Operations Office  
**Website:** www.inl.gov

- **FY 2016 Lab Operating Costs:** $1,034 million  
- **FY 2016 DOE/NNSA Costs:** $852 million  
- **FY 2016 SPP (Non-DOE/Non-DHS) Costs:** $182 million  
- **FY 2016 SPP as % Total Lab Operating Costs:** 21%  
- **FY 2016 DHS Costs:** $35 million

**Physical Assets:**
- 569k acres and 534 buildings  
- 2.3M GSF in buildings  
- Replacement Plant Value: $4.8B  
- 69k GSF in Excess Facilities  
- 1M GSF in Leased Facilities

**Human Capital:**
- 4,272 Full Time Equivalent Employees  
- 20 Joint Faculty  
- 41 Postdoctoral Researchers  
- 105 Graduate Students  
- 198 Undergraduate Students  
- 72 Facility Users  
- 470 Visiting Scientists

**FY 2016 Costs by Funding Source ($M)**

- NE $489.0  
- EERE $36.0  
- NNSA $210.0  
- DOD $119.0  
- DHS $35.0  
- DOE Other $82.0  
- Non Fed SPP $22.0

**Mission Overview**

Idaho National Laboratory (INL) is America’s lead nuclear energy laboratory. Its mission is to discover, demonstrate, and secure innovative nuclear energy solutions, other clean energy options, and critical infrastructure. INL achieves these mission objectives and technical outcomes and executes INL’s vision to change the world’s energy future and secure critical infrastructure through:

- Focus research and development (R&D) on grand challenges in energy and national security.
- Designing, building, and operating world-class and unique research, development, and demonstration (RD&D) infrastructure, making these resources available to universities and industries to innovate—in partnership with INL—our R&D network.
- Working toward creating a global nexus of world-class research and engineering talent.
- Building and sustaining global strategic partnerships.

To execute the INL mission, INL integrates and applies distinctive core capabilities and unique R&D facilities with signature strengths in nuclear energy, clean energy deployment, and modernizing and securing critical infrastructure. The outcome will be transformational innovations in energy and security concepts.
In operation since 1949, INL is the nation’s leading R&D center for nuclear energy, including nuclear nonproliferation, physical and cyber-based protection of energy systems and critical infrastructure, and integrated-energy-systems. INL has been managed and operated by Battelle Energy Alliance, LLC (BEA), a wholly owned company of Battelle; for the Department of Energy (DOE) since 2005. BEA is a partnership of Battelle, BWX Technologies, Inc.; AECOM; the Electric Power Research Institute (EPRI); the National University Consortium (comprising Massachusetts Institute of Technology, The Ohio State University, North Carolina State University, University of New Mexico, and Oregon State University); and the Idaho University Collaborators (University of Idaho, Idaho State University, and Boise State University).

Core Capabilities

Of the 24 core capabilities distributed across DOE’s science and applied-energy laboratories, INL has 13 DOE acknowledged core capabilities and two DOE-acknowledged emerging core capabilities, indicating the exceptional breadth of its scientific and technological foundation. This represents a science and engineering skillset that extends across a continuum, connecting basic and applied research to testing, demonstration, and deployment. INL offers a broad array of capabilities in both fundamental and engineering sciences in support of the DOE mission, and the Laboratory delivers critical outcomes in nuclear, clean energy and environment systems innovation and integration, and critical infrastructure protection. Appendix C maps INL core capabilities to DOE programs.

INL’s core capabilities span nuclear engineering and related scientific disciplines, such as applied materials science, chemical and molecular science, condensed-matter physics and materials science, nuclear and radiochemistry, chemical engineering, systems engineering, decision analysis, and probabilistic risk assessment, as well as purpose-built research infrastructure for nuclear energy, at-scale clean energy and environmental-technology deployment studies, and critical infrastructure protection. Each core capability is a substantial combination of knowledge, people, equipment, and facilities, having unique and/or world leading components, and is employed to respond to the INL mission challenges for DOE, the National Nuclear Security Administration (NNSA), the Department of Homeland Security (DHS), the Department of Defense (DoD), the National Aeronautics and Space Administration (NASA), and other INL customers. Capability synergies enable INL to address challenges posed by DOE to carry out the transformative research required to accelerate the delivery of energy, environmental, and security solutions to the marketplace, with an emphasis in R&D. INL’s research, development, demonstration, and deployment (RDD&D) capabilities, resources, and unique geography enable the integration of scientific discovery, innovation, engineering, operations, and controls into complex, large-scale test beds, and demonstration platforms for discovery, innovation, and demonstration of at-scale transformational energy and security concepts.

Created as the National Reactor Testing Station, INL pioneered the first nuclear generated electricity to power an American community (Arco, Idaho) and demonstrated the Navy’s first nuclear propulsion systems. INL is where the nation’s best and brightest researchers and engineers come to advance the promise of nuclear energy, the most reliable and cost effective energy source to enable national objectives for addressing climate change. Since its creation, INL’s RDD&D portfolio has expanded. Today, INL is the lead national laboratory for nuclear energy RD&D, supporting the long-term operations of commercial light-water reactors (LWRs), designing and developing advanced nuclear reactors and associated fuel cycles and nuclear fuels and materials, coupling experiments with modeling and simulation to design materials and systems for accelerated development, demonstration, and deployment of nuclear energy technologies. INL is home to some of the world’s unique facilities that support innovations across all aspects of nuclear energy and national security. In addition to nuclear energy, INL is a globally recognized R&D leader in control systems cybersecurity and makes important
contributions to secure and modernize the nation’s critical infrastructure, including an emphasis on cybersecurity protection of the national power grid and nuclear energy facilities.

INL’s 890 square mile laboratory and testing complexes represent a synergistic integration of co-located and networked nuclear and national security facilities. INL hosts unparalleled assets, such as the Materials and Fuels Complex (MFC); the Advanced Test Reactor (ATR); the Transient Reactor Test Facility (TREAT); a utility-scale electric-power grid for improving grid reliability and security; a wireless communications test bed supporting commercial and government-sponsored research; key capabilities for performing cyber and control-system research, explosives and ballistic threat analysis, and armor development and production; and safe and secure locations for accelerating protective-solutions development and testing, as well as for facilitating first-responder training experiences in nuclear forensics, real-world contamination scenarios, and incident response. Combined with its internationally recognized critical infrastructure protection and nuclear-nonproliferation scientists and engineers, the INL resembles a city/region where challenging energy and security questions can be answered at scale.

INL is focused on achieving full value of all energy sources by coupling nuclear energy with both the grid and industrial manufacturing via heat and electricity with carbon resources, including CO2, biomass, coal, natural gas, and other petroleum resources. This coupling will enable fission-generated radiation and heat to drive industrial processes in addition to reliably generating electricity in decentralized, hybrid energy systems (HESs). INL has also made significant contributions in renewable-energy grid integration and transportation-system transformation. INL’s R&D continue to advance energy-intense processes with the switchable-polarity solvent forward osmosis (SPS-FO) capability, which provides a novel means to purify water, electrochemical conversion science to reduce the temperatures necessary to conduct specific chemical conversions, and separation science to recycle valuable rare-earth metals. INL is developing technologies that increase the balance, diversity, efficiency, affordability, and accessibility of domestic sources of energy and supporting the national transition to industrial competitiveness through energy security.

INL applies core capabilities to non-DOE customer needs through Strategic Partnership Programs (SPPs) and other mechanisms that contribute to DOE’s mission achievement. SPPs also strengthen INL capabilities and sustain the ability to deliver on DOE missions.

1. Applied Computer Science, Visualization, and Data

INL’s strategic intent is sustained leadership with advances in applications in computational science and engineering, specifically focused on applications in nuclear and clean energy, and critical infrastructure protection R&D. INL’s computing success has been the rich internal and external collaboration centered on the Multiphysics Object Oriented Simulation Environment (MOOSE) framework. INL created MOOSE, an open source, high-performance computing (HPC)-based simulation framework. with significant investment of LDRD funds. The framework was built on a unique computational science approach, combining computer science with a mathematical description of physics. MOOSE enables domain scientists to rapidly obtain fully coupled, fully implicit solutions of multiphysics problems using state-of-the-art nonlinear/linear solvers and takes full advantage of massively parallel computing. BISON (Broadly Implicit Simulation of Nuclear fuel), a MOOSE-based simulation tool, supported by the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program, has been developed to predict the behavior of nuclear fuels and materials undergoing irradiation for nuclear reactors under both normal operating and accident conditions. National and international laboratories and universities have developed more than 40 MOOSE-based applications.

INL focuses on advancing MOOSE-based software applications for nuclear power, materials, structural dynamics, multiphase flow, waste analysis, and geophysics. Nuclear power applications include radiation transport, reactor physics, nuclear plant safety and systems analysis, growth and effects of corrosion
and wear products (e.g., rust and particles), and multiscale nuclear fuels performance. Materials applications include materials development, effects of corrosion, damage and aging evolution, and irradiated material analysis. Over the years, MOOSE has evolved as a general-purpose, multiscale, multidomain simulation framework in many fields, including subsurface reactive-transport modeling and coupled hydro-thermo-mechanical-chemical processes. For these reasons, INL is a recognized leader in the development of models to better understand fractures and fluids in tight rock formations, safe long-term stewardship of chemical- and nuclear-waste disposal in the subsurface (numerical simulation of contaminant fate and transport), risk analysis, and performance assessment. Geophysics applications include seismic, geothermal, geochemistry, and isotope transport. MOOSE’s unified computational framework is also ideally suited for the development of next generation earth-system models, which require multidomain, multiscale, multiphysics coupling among hydrological, biological, and geochemical processes across both the subsurface environment and terrestrial ecosystems. INL will enable an increasing number of MOOSE-based applications, coupling experimental studies with modeling and simulation, and enhanced validation of these predictive capabilities through investment in a Collaborative Computational Center. INL’s risk-informed safety-margin characterization is supported by the MOOSE-based safety-analysis tool and supports management of uncertainty, nuclear reactor design, and improved decision making for nuclear power plants. ATR modeling and simulation (M&S) advances computational methods for nuclear-reactor design/analysis. Integrated reactor experiments and M&S are achieved through the TREAT simulator.

INL has also been successful in developing and applying computing and analytical innovations in order to enhance the security of critical infrastructure. Many of these innovations have immediately been put into practice by a variety of analysts and stakeholders in the critical infrastructure protection community, including DOE, state and local governments, infrastructure owners and operators, and in particular, the Department of Homeland Security. Examples include the All Hazards Analysis Framework used to mitigate vulnerabilities from dependent infrastructures. This innovative approach develops dependencies profiles and complex geospatial analyses. Innovative techniques are also being applied to the analysis of cyber infrastructure through geospatial representation and analysis. This is driving INL more to the forefront of big data analytics and data-intensive computing.

Approximately 80 researchers, including four joint appointees and 13 postdoctoral researchers with expertise spanning physics, applied mathematics, materials engineering, mechanical engineering, risk analysis, computer science, computational science, and nuclear reactor engineering support this core capability. INL’s Scientific Computing group provides computing and visualization resources to develop new capabilities, build tools, foster collaboration, and support external users. HPC systems run application codes from three primary categories: user-developed and open-source codes, such as MOOSE; DOE-controlled nuclear software, such as MCNP, ORIGEN, SERPENT, and MC21; and commercial engineering and scientific codes, such as STAR CCM+, Abaqus, and VASP, which are used in research involving computational fluid dynamics, structural analysis, and materials modeling.

Computer M&S, when appropriately validated and coupled with experiments, extends understanding beyond some of the limitations of experiments. In complex systems, such as a nuclear reactor or a power-distribution grid, the theory that governs the behavior of individual components becomes interconnected in complex ways that both theory and experiment struggle to fully capture, predict, or explain. In these instances, computer modeling and simulation can provide critical insights and help accurately develop the understanding needed to engineer, design, research, and operate very complex systems. Nuclear energy development efforts have historically relied largely on theory and experiment, but in the future will rely increasingly on computer modeling and simulation. The field of big-data analytics and data-intensive computing is a relatively new core capability that has significant applicability to many INL areas, such as knowledge management and validation, national security programs, cybersecurity research, and earth and environmental sciences.
INL has leveraged this capability to support programs for the Office of Nuclear Energy (NE), Environmental Protection Agency (EPA), DoD, EPRI, Westinghouse, AREVA, Geothermal Technologies Office, the Office of Energy Efficiency and Renewable Energy’s (EERE’s) Bioenergy Technology Office, DHS, and NNSA. This capability advances DOE’s goals in science and energy and nuclear security, as articulated in the DOE Strategic Plan.iv

2. Applied Materials Science and Engineering

Through its core competency in applied materials science and engineering, INL is recognized as an international leader in nuclear energy research, a national leader in critical infrastructure protection, and the U.S. Army’s Armor Center of Excellence. INL provides a technical basis for the development and qualification of materials, material systems, and processes for a range of nuclear-reactor applications, armor protection, hardening of critical infrastructure, and emerging energy systems through a multiscale understanding of physical and mechanical properties. An integrated set of capabilities, ranging from nanoscale discovery to national code-case development, allow INL researchers to fabricate, characterize, and test energy materials, including nuclear fuels and materials, at quantities spanning experimental to prototypic scale. INL’s research expertise is in advancing nanoscale chemistry, understanding dislocation dynamics and nucleation and growth phenomena; and characterizing materials. This expertise is used to resolve complex mechanisms and understand the relationships between structure and properties, the role of defects in controlling properties, allowing improved performance of deployed materials in the most hostile environments and extreme-dynamic loading environments.

Increasingly, research and experimental efforts are strongly coupled with INL’s modeling and simulation capabilities at the macro- and mesoscales. Sophisticated equilibrium- and kinetic-modeling tools are used to design materials and systems for nuclear energy, armor, and critical infrastructure protection. The MOOSE-BISON-MARMOT platform is an internationally adopted multiscale, multiphysics, three-dimensional, finite-element, transient and steady-state framework that allows easy development of application software with emphasis on developing fuel performance codes based on first-principles science with less reliance on empirical models. The Armor Research and Engineering Institute integrates established material applied R&D, modeling and simulation, prototyping and testing, and evaluation capabilities available across INL to provide technical advancements in weight, space, and cost-effectiveness of armor for personnel, vehicles, and facilities against the full spectrum of ballistic and explosive threats.

The strategic intent of the applied material science core competency is to: (1) develop coupled testing and characterization approaches to enable intelligent design of materials and predict property evolution under extreme conditions; (2) facilitate refinement of international evaluations and test standards; (3) develop and apply advanced instrumentation capabilities that allows in-situ measurement of material response in extreme environments; (4) develop the next generation of verification, signatures, and observables for the safeguarding of nuclear and radiological materials; and (5) develop the next generation of armor materials to defend the nation. INL will continue to develop and improve modeling and simulation, material fabrication, characterization, and testing capabilities aimed at smart material and system design. This will shrink product development cost and ensure a more responsive product-development cycle.

The combination of large-scale facilities at ATR, MFC, and TREAT, the Specific Manufacturing Capability (SMC) and complementary capabilities at the Center for Advanced Energy Studies (CAES), Energy Innovation Laboratory (EIL), and National Security Test Range makes for world-class materials RD&D capability. The U.S. Navy, for example, has used these capabilities to develop life-of-the-ship submarine reactor cores.
Approximately 481 staff members and 12 postdoctoral research associates support this core capability. INL holds 27 patents in this area. Primary customers for this capability are NE, EERE, Office of Electricity Delivery and Energy Reliability (OE), SC, NNSA, DHS and DoD. Other customers include EPRI, TerraPower, Westinghouse, Office of Naval Reactors (NR), the Korea Atomic Energy Research Institute (KAERI), and the intelligence community. In addition, INL is working toward sponsorship from the Nuclear Regulatory Commission (NRC), DHS, Basic Energy Sciences, the Department of State, Advanced Research Projects Agency-Energy, U.S. Army Tank-automotive and Armaments Command, U.S. Army Program Executive Office Ground Combat Systems, and the U.S. Army Tank-Automotive Research, Development, and Engineering Center.

3. Biological and Bioprocess Engineering

INL’s core capability spans bench-top analysis through scale-up and integration to address challenges in biomass preprocessing solutions, logistics, feedstock-supply specification, supply-chain development, and demonstration challenges. INL focuses on innovation in feedstock and bioproducts to incorporate bioenergy as a viable part of an energy portfolio. INL performs independent analysis, development, and scale-up of preprocessing systems with producers of biomass feedstock and bioproducts to reduce variability and produce high-quality feedstock from grass, wood, and agricultural residues. Biomass variability makes a uniquely challenging feedstock compared to other energy feedstocks, such as coal and crude. Over the last decade, INL has built expertise in characterizing chemical and mechanical properties, decontamination process technology, trace detection, and process-system design. INL is recognized by EERE’s Bioenergy Technologies Office in supporting two priority areas: (1) feedstock-preprocessing scale-up and integration and (2) feedstock production and supply.

The strategic intent is to mobilize the nation’s diverse and variable biomass resources by reducing delivered cost and risks associated with feedstock quality and volume and accelerating widespread commercialization of sustainable biomass supply chains for a broad range of markets.

INL applies expertise in systems integration, chemical engineering, analytical chemistry, agricultural science, and materials science to feedstocks. We apply these to develop the science of supply chain scale-up and integration to produce consistent, conversion-ready feedstocks that improve reliability and operability of biorefinery technologies. INL combines operational data and field trials, physiochemical-characterization data, and laboratory- and full-scale conversion data to: (1) inform feedstock development and selection, (2) improve conversion-process development and selection, (3) streamline supply-chain processes, (4) assess the value of domestic and export trade, (5) develop U.S. biomass standards, and (6) utilize a large-scale, fully integrated pilot facility for process development, scale-up, and toll processing.

INL is expanding this capability by developing particle mechanics and solids flow capabilities with expanded computational science tools, such as computational fluid dynamics and discrete element modeling supported by HPC capabilities. Enhanced characterization tools (e.g., nuclear magnetic resonance, microscopy, and quantitative 3D X-ray), mechanical-testing tools (e.g., flowability analysis and shear testing), and large-scale validation is performed in the process-demonstration unit (PDU) to support many scientific opportunities. We are also expanding the large-scale infrastructure capabilities of the Biomass Feedstock National User Facility (BFNUF) PDU to include additional process science and technology options for broader applicability to industry scale-up and integration needs. The BFNUF represents a world class capabilities in solid materials handling and preprocessing at INL. As the capabilities are developed, they will be available through the BFNUF to support collaborative projects that may include regional or national partners from industry, universities, and other federal agencies. In particular, INL has worked with DOE-BETO on several equipment upgrades to improve the relevance and value of those capabilities to the national user community. Additionally, efforts to improve business processes and technical offerings (including partnering with other DOE national biomass centric
laboratories) are expressly focused on increasing the facility utilization, by which increased utilization reduces individual user’s costs (including DOE’s) and stabilizes the long-term viability of the asset.

Approximately 110 staff members support this capability, including experts in chemical engineering, materials science and engineering, systems science, data mining, computational intelligence, and cognitive learning approaches. INL’s enduring physical asset and the flagship of the BFNUF, the PDU, is a one-of-a-kind, fully integrated pilot facility. The PDU’s innovative design—modular and reconfigurable—helps bioenergy companies find the best way to convert feedstock into fuel. Capable of processing anywhere from two to five tons of biomass per hour, the PDU is a unique tool to accommodate the varied needs of process design and feedstock supply. While the PDU is the associated biomass-processing capability of the BFNUF, other components, like the Bioenergy Feedstock Library and the Characterization Laboratory, make this arguably the most complete feedstock preprocessing R&D and pilot facility in the world.

The primary customer is EERE for bioeconomy development, with INL responsible for specific strategies and outcomes, as identified in the Bioenergy Technologies Office’s strategic plan. INL has and continues to make significant facilities investments in the biomass program. Recent investments include: covered storages for Biomass product(s) behind the PDU facility bay, additional laboratory bench space in the EIL (across the street from the current biomass laboratory) is readily available and HPC/visualization resources for particle mechanics projects have been added to enhance the scientific offerings to sustain this INL capability. In addition, INL’s expertise in material processing, feedstock development for biopower and bioproducts, and machine learning and process control make these capabilities relevant to the needs of the Office of Fossil Energy (FE), Advanced Manufacturing Office, and other federal interests, as well as various state initiatives in energy efficiency.

4. Emerging: Chemical and Molecular Science

Over the years, INL has developed expertise in understanding, predicting, and controlling physical and chemical transformations and has created a robust knowledge of chemical process technologies that encompasses expertise in membrane and filtration science, electrochemical processing and separation, supercritical fluid science, interfacial and surface science, radiochemistry, actinide chemistry, catalysis, and trace analytical measurements to support holistic efforts to enable the next generation of processes that lower energy consumption, secure supplies of critical energy materials, and reduce waste.

INL has applied chemical and molecular science to develop scientific advancements that improve both energy- and resource-intense processes. Facilities that support this capability include the EIL, CAES Materials and Characterization Suite (MaCS), and the Energy Systems Laboratory (ESL). Most recently, INL has developed capabilities in temporal analysis of products (TAP) for catalysis research, which is a novel technique to probe reaction kinetics of gas-solid interactions, SPS-FO for water purification, electrochemical carbon utilization and hydrogen production, subsurface interfacial science, and rare earth recycling and reuse.

The TAP capability is unique within the DOE complex, and INL is one of only two with the capacity in the U.S. TAP is being used to assess steps of elementary reactions on complex materials (as opposed to single crystal surfaces) for development of multistep microkinetic reaction mechanisms. TAP requires specialized expertise for design, execution, and interpretation of experimental data. INL’s team is positioned to develop new materials for high-energy-intensity processes. The TAP combines scale-up process modeling and reactor development with an industrial consortium. The goal of the consortium is to integrate industrial involvement in development activities that shorten the time required to adopt new approaches and help coordinate activities that result in measurable impact.

Inherent to the TAP and its industrial consortium is CAES, where the TAP instrument is located. CAES is a modern 55,000 square foot facility that fosters multi-institutional, collaborative energy-research
programs important to the nation. It attracts students and faculty, promotes informed energy policy
dialogue across Idaho and the nation, and acts as a focal point for technology-based economic
development in Idaho. In addition to TAP, CAES includes laboratories supporting a number of research
capabilities: (1) radiochemistry, (2) advanced materials, (3) analytical chemistry, (4) advanced
transportation, (5) microscopy and characterization, (6) fluid dynamics, (7) advanced visualization, (8)
analytical instrumentation, and (9) human-performance simulation. The capabilities are made available
through collaborative research activities in nuclear science and engineering, bioenergy, carbon
management, energy efficiency, and advanced materials.

Science-based advancements continue to enhance energy-intense processes with the SPS-FO capability,
which provides a novel means to purify water. SPS-FO technology can be operated using waste heat or
cheap, high-grade thermal heat from sources such as natural gas. By removing the need for significant
electricity inputs, the cost of water treatment can be significantly lowered using SPS-FO in place of more
traditional processes, such as reverse osmosis. This enables targeted, cost-effective water reuse that, in
turn, can result in processing with zero liquid discharge. This is of significant value for water-constrained
regions in the U.S., where availability is also a driver, along with the cost of supply and treatment. An
example is the Northwest region, where agriculture and the food-processing industry have a significant
economic footprint. There is substantive regional engagement with INL in water recovery and reuse. An
additional parallel benefit of this technology is its applicability to the energy industry. Currently, INL is
working on developing a joint project with a nuclear utility to adapt SPS-FO technology to the needs of
thermal cooling and water upgrading. If successful, this work could alleviate the need for additional
holding ponds on the site of the utility, which is highly desirable in terms of both cost and environmental
impact.

Electrochemical-conversion science has been developed that reduces the temperature necessary to
conduct specific chemical conversions. Lower temperatures equate to lower energy consumption. For
example, a direct carbon electrochemical-cell technology has been developed that can use a variety of
hydrocarbon resources, including inexpensive natural gas or biomass, to generate hydrogen at low
temperatures. Another example is the activation of CO2, which allows the gas to be used as a feedstock
for higher-order, value-added chemicals, rather than the conventional impression that CO2 is a waste
by-product. Also, this technology has been developed to take advantage of available energy resources,
consistent with the hybrid energy-systems concept, through its ability to be integrated with the
electrical grid. Integral to these electrochemical approaches is the ability to examine and characterize
interfacial phenomena. This can include catalyst or electrode surfaces, but also has application in the
subsurface. For example, expertise has been built that can characterize the fundamental interactions
between subsurface organics (fluids, kerogens) and inorganic geological strata. These fundamental
abilities are conducted at the nanometer scale so that they are able to provide insight into fluid
dynamics and adsorption into nanometer-scale pores in the kerogen material, a process which
influences the fate and transport of subsurface species.

Significant capabilities for separation science have been developed to recycle valuable rare-earth
metals. Supported by the DOE Critical Materials Institute, technologies have been developed to
selectively isolate rare-earth elements (REEs) from complex mixtures. Differentiating capabilities include
supercritical fluid extraction using benign solvents, electrochemical deposition of selected metals (both
REEs and precious metals) onto an electrode surface suitable for product isolation, and biological
complexation, where microorganisms with specific binding tags have been shown to be effective in the
isolation of REEs from acidic solutions.

The capability is supported by approximately 111 staff members with expertise in materials science and
chemical engineering, and is expanding capabilities in (1) process design and scale-up; (2) carbon
conversion; (3) carbon-feedstock (biomass, CO2) separation and characterization; (4) chemical
compositional analysis; (5) thermochemical feedstock properties; (6) rapid screening techniques; (7)
microscopy and imaging; (8) particle characterization; (9) post-irradiation examination (PIE); (10) nondestructive analyses; (11) actinide and rare-earth chemistry; (12) advanced electrolysis and corrosion; (13) surface-analysis technologies; and (14) systems engineering.

Primary customers for this capability are NE, EERE, OE, and DoD. In particular EERE-Geothermal Technologies Office (GTO) and DOE Advanced Manufacturing Office are funding efforts with the SPS-FO and TAP respectively. The SPS-FO efforts and Water Security Test Bed activities are a demonstration of INL’s chemical and molecular science activities. DOE-FE currently funds a project associated with purifying CO₂ for potential use as a chemical feedstock. The EPA is funding efforts at INL’s Water Security Test Bed. Both agencies have been engaged in exploring future R&D opportunities. INL is actively working to increase its SC collaborations and partnerships. Most recently, industrial interest in the TAP consortia has been received from DOW Chemical, DuPont, BASF, Shell, and Grace.

5. Chemical Engineering

INL has extensive chemical engineering capabilities, developed since the early stages of the Laboratory’s missions and programs, related to nuclear fuel separations, radioactive waste treatment, energy-intensive industrial and clean transportation process transformation, catalysis development, critical energy materials purification and recovery, polymer synthesis, and energetics and reactive materials prototyping.

The Laboratory’s history and expertise in reprocessing spent nuclear fuel (SNF) provide unique capabilities in process chemistry and development for separation of highly radioactive chemicals using aqueous solvent-extraction technology or by nonaqueous electrochemical means. INL is the only laboratory in the U.S. that has engineering-scale pilot plants to perform testing with all three major solvent-extraction equipment types (pulse columns, mixer-settlers, and centrifugal contactors); electrorefining; biofeedstock; and test facilities and ranges for experimentation and testing of energetics, reactive materials, and Ballard protection (ceramic, polymeric, and metallic) systems. These pilot facilities currently support development of separation technologies for nuclear energy, critical materials, renewable-energy, environmental management, and national security missions. INL is also the only lab in the U.S. that has an engineering-scale electrochemical separations facility for processing used nuclear fuel. INL engineers have successfully demonstrated the scale-up of electrochemical processing by three orders of magnitude. This facility continues to play a key role in the exploration of safeguards and advanced separations processes and is an important element of U.S. cooperation with the Republic of Korea.

The chemical engineering capability also reaches into non-nuclear areas. INL is a technical leader in developing solid-oxide cells for the production of hydrogen and synthetic gas using heat and electricity. INL has six test stands for long-duration, unattended experiments on single cells and on stacks containing three to 25 cells. Its longest test has lasted 2,500 hours, and its largest test included 720 cells and 18 kW. INL’s expertise in identifying and characterizing chemical constituents in extremely harsh environments is used to understand how materials withstand highly corrosive, high-temperature environments typical of those required for thermochemical production of hydrogen, production of synthetic fuels, and removal of carbon dioxide from chemical processes and power plant exhaust.

INL partners with U.S. industry, area universities, and other national laboratories to actively develop safe, high energy storage lithium batteries; new, efficient methods for optimizing biomass for conversion to bioenergy, biofuels, and other bioproducts; novel biochemical routes to renewable fuels; durable storage materials for processing, transporting, and storing nuclear waste; efficient methods for recycling energy-critical materials; and safe, energetic materials for national security applications.

INL’s projects demonstrate expertise in several additional areas, including applied chemical and industrial-process modeling, systems engineering, system-control theory, chemical synthesis, catalysis,
super-strong and ultra-hard materials, and radioactive waste treatment. The strategic intent is to lead market transformation through advanced chemical separation and heterogeneous chemical and electrochemical catalysis, advanced process engineering, and materials integration by bringing vital research to scale. INL’s expertise in applied chemical and industrial-process modeling, systems engineering, and system-control theory provides a unique ability to integrate complex chemical operations. INL’s newly established Dynamic Energy Transport and Integration Laboratory offers unique capabilities to assess the complexity of nuclear, fossil, and renewable HESs for both transportation and manufacturing.

Facility upgrades consistent with mission needs are further discussed in Section 4. Investment is needed to maintain existing capabilities (including intellectual resources) at the state-of-the-art level in this quickly evolving field.

Approximately 125 staff members support this capability at MFC, Bonneville County Technical Center, Idaho Nuclear Technology and Engineering Center (INTEC), Moran Pilot Plant, Remote Analytical Laboratory CPP-684, MaCS, CAES, ESL, and EIL.

Primary customers for this capability are missions related to nuclear energy, environmental management, efficient and renewable energy, and national and homeland security. Major funding comes from DOE (NE, EM, NNSA, and EERE); NHS; and DoD.

6. Emerging: Condensed-matter Physics and Materials Science

INL’s core capability in condensed-matter physics and materials science is aimed at developing a comprehensive, atomic-to-mesoscale understanding of material behavior in extreme environments with the ultimate goal of more efficiently capturing the energy in the nuclear bond. This capability, which underpins INL’s nuclear energy mission, is closely tied to a computational materials-science modeling effort (see Section 3.1, “Applied Computer Science, Visualization, and Data”). Active areas of research include:

- Investigating the coupling between various degrees of freedom (charge, lattice, spin, and orbital) and the interplay with strongly correlated ground states, such as complex magnetism and superconductivity, in 5f electron materials
- Utilizing radiation to drive the self-organization of patterned nanostructures
- Investigating radiation-induced defect formation, clustering, and elemental redistribution
- Using coherent acoustic phonons to probe subsurface structure and function of grain boundaries
- Investigating mechanical properties of materials with respect to extremes in radiation, temperature, and pressure
- Connecting the science of defects and thermal transport in nuclear fuels
- Using mechanical spectroscopy to monitor microstructural evolution at high temperatures.

As part of this core capability, INL is providing the nuclear science community access to world class capability to characterize irradiated materials. Resources include laser-based characterization of thermal and mechanical properties, state-of-the-art microscopy and tomography at the meso- and atomic-scales, and new capabilities in temperature, magnetic field, and pressure-dependent magnetometry, thermodynamics, and transport. The combination of these distinctive experimental capabilities and staff competencies make INL a unique place to perform research on actinide-bearing materials.

INL is also developing a new in-pile instrumentation capability that will provide real-time, accurate, spatially resolved information regarding performance of fuels and materials that can be directly tied to microstructure. As these capabilities mature, scientists will have unprecedented access to the time-dependent, in-reactor environment (temperature, pressure, flux, etc.) and will be able to monitor
material behavior that cannot be captured in a post-irradiation environment. These new instruments represent a step change in capability over current in-pile instruments and will require developing sensor materials that are resistant to radiation, chemical diffusion, and thermal and mechanical stresses. These new experimental tools will be complemented by the state-of-the-art computational materials science models.

Approximately 90 staff members, including two joint appointees and five postdoctoral researchers, support this capability to address challenges in condensed-matter physics. Our research utilizes on-site state-of-the-art facilities (such as the Electron Microscopy Laboratory, Irradiated Material Characterization Laboratory (IMCL), CAES MaCS, laser-based materials characterization laboratories, a physical-property measurements laboratory, and the Carbon Characterization Laboratory) as well as a variety of off-site collaborations and cutting-edge user facilities, such as the National High Magnetic Field Laboratory, Advanced Photon Source, and Actinide User Laboratory at the Institute for Transuranium Elements in Karlsruhe, Germany. Primary customers for this capability include programs for NE, Basic Energy Science program, NNSA, and NR.

7. Cyber and Information Sciences

Cyber and information sciences are the disciplines, technologies, and practices designed to protect, analyze, and disseminate information from electronic sources, including computer systems, networks, and sensors. Expertise areas are typically cybersecurity, information assurance, information analytics, knowledge representation, and information theory. In the realm of control systems cybersecurity, there are the added complexities of physical effects, systems- and engineering-control theory, embedded processing, and unique forms of digital protocols, all used in combination with computer information systems. The science and engineering of control systems within cyber-physical systems includes protection against adverse effects (e.g., from electromagnetic, mechanical, and chemical forces), interdependency analysis, and cybersecurity, and is a unique multidisciplinary domain that INL is helping to define for the nation. Our aspiration is to develop the science and fundamental methods to redesign control systems to increase resiliency, not only during natural and incidental events, but also under cyber attack. The next generation of control systems used in critical systems must provide situational awareness of adversaries, autonomously mitigate adversarial effects, and enable restoration to safe and trusted operation.

The Cybercore Integration Center, an INL critical outcome, seeks to provide the nation with an enduring cyber-physical innovation capability that specifically leverages this core capability. Scientific explorations include the systematic crossover into cyber and information sciences; decision science; applied, mechanical, and system engineering; visualization; etc. The resulting discoveries will lead to advanced engineering tools and assessment methodologies for cyber-informed designs, new sensor systems, algorithms for advanced analytics-based resiliency decisions, next generation cyber-immune network and communication architectures for control systems, and real-time simulation and emulation systems for event planning, response, and recovery.

INL is an internationally recognized leader in control systems security within the strategic confluence of cyber and infrastructure security, embedded controls, wireless communications, vulnerability processing, and technical threat analysis. Over two decades of multidisciplinary teaming for the security and resilience of critical infrastructure against all hazards, with an emphasis on cyber/physical threats and inherent interdependencies, has provided INL with a unique foundation of expertise and infrastructure capabilities in the specialized science of control systems cybersecurity.

INL’s multidisciplinary teams represent the top talent for evaluation of technical threats and threat actor analysis, vulnerability assessment, interdependency and impact analysis, prototype and solutions/products development, demonstrations, and technical training. INL provides leadership and
expertise for both private industry and federal programs, as illustrated by the 10-year success of Resilience Week, an annual INL-sponsored symposium, held in conjunction with the Institute of Electrical and Electronics Engineers and myriad universities, dedicated to transforming the resilience of cognitive, cyber-physical systems. INL’s approximately 250 cyber- and information-sciences staff members have broad expertise spanning critical infrastructure testing and analysis, control systems cyber R&D, infrastructure resiliency, sector control systems, communications, cyber-informed design, and disaster recovery for national agencies such as DHS, DOE, NNSA, the International Atomic Energy Agency (IAEA), DoD, and the Department of Justice. INL maintains strong relationships with control systems vendors, cyber-physical researchers, and infrastructure owners or operators, as well as universities that are training researchers in this field (e.g., University of Idaho, Idaho State University, Boise State University, University of Tulsa, and New Mexico Institute of Mining and Technology).

INL’s R&D capabilities and long-standing support of the DHS National Cybersecurity and Communications Integration Center (NCCIC) is an example of how INL’s expertise in vulnerability discovery, malware analysis, incident response, risk assessments, reverse engineering, and hardware exploitation support the control-system security needs of the nation. In addition to this support, INL advances methodologies and tools utilized by NCCIC, such as Automated Vulnerability Assessment and All-Hazards-Analysis R&D, which increase the scalability of critical infrastructure assessments and enable the development of a catalog of critical systems for rapid evaluation. These capabilities are applied to other DHS programs supporting activities in regional resilience, infrastructure situational awareness, and infrastructure dependencies and interdependencies.

INL’s cyber R&D innovations have been validated through 17 U.S. patents awards, 13 copyright assertions, two open-source software releases, and more than 100 publications and conference presentations. Specific innovations within the fundamental science of intelligent monitoring and control include: (1) cyber-state awareness in trusted control loops, (2) cyber-monitoring techniques for unique and fragile protocols in operational layers of controls systems, (3) techniques and tools for embedded control systems forensics and verification, and (4) out-of-band sensors, operational-process modeling, and fusion of sensors and state models into operational cyber-situational awareness.

INL provides international and domestic leadership in nuclear cybersecurity across the commercial (nonweapons) fuel cycle and leads the innovation in cyber-informed engineering of control systems and reprioritizing R&D and mitigation activities founded on risk-based analysis of cyber-physical consequence. Aligned within the strategic objectives of nuclear cybersecurity research programs of DOE-NE and NNSA, INL is serving as a leader in the advancement of a framework for enhancing the cybersecurity of nuclear facilities. This framework includes strategies for cyber-informed engineering, advanced malware detection, forensics analysis, reverse-engineering, and attack mitigation and response. At the request of the IAEA, INL cybersecurity subject matter experts have assisted in updating design-basis threat guidance, conducted in-field technical training, and teamed with other international experts to produce direction related to conducting cybersecurity training and assessments of nuclear facilities.

In addition, INL’s cyber and information sciences core capability supports DOE’s mission by developing technologies that use computational intelligence methods to address complex engineering issues. For example, INL introduced innovative monitoring and decision-making technologies for effectively integrating complex energy systems and increasing their energy-conversion efficiency, decreasing environmental impact, exploiting low-quality energy sources, enabling efficient grid introduction of intermittent renewables, managing variability, enabling resiliency behavior, improving safety, and accommodating reliable and stable dynamic operation. To improve national security, INL has likewise developed predictive techniques that can best utilize collected information to allow prompt detection, diagnostics, prognostics, and control of anomalies and to monitor health conditions of equipment, unit operations, processes, systems, and systems-of-systems under observation.
Primary research and experimentation facilities include: Critical Infrastructure Test Range Complex (CITRC), National Electric Research, Test, and Evaluation Grid, Smart Grid Communications Test Bed, Substation Controller Test Beds, Wireless Test Bed, Water Security Test Bed, and the Control System and Cybersecurity Innovation Laboratories, including embedded reverse-engineering, digital real-time simulation, transportation systems, electric vehicle charging, and wireless chambers. Myriad infrastructure is available for full-scale testing (of transportation, chemical-processing, biofuels, and manufacturing). DHS mission-related facilities include the NCCIC watch floor, Advanced Analytics Lab (performing malware forensics), incident responders and fly-away teams, industrial-scale training facilities, and a collection of testing and assessment systems.

8. Decision Science and Analysis

Decision science and analysis is a subdiscipline of systems analysis. It derives insights from experimental data and modeling and simulation results to further the understanding of resource and technology options; to identify and quantify the risks, uncertainties, and impacts of current and emerging technologies; and to assess the impact of market dynamics, human behavior, regulations, policies, and institutional practices on decisions. This capability provides credible information to assist DOE and other government agencies, regional stakeholders, and programs with strategic planning and program direction, policy formulation and implementation, and efforts to remove market barriers to deployment and to improve engagement with stakeholders. INL is a leader in data-driven methods, probabilistic modeling, complex systems analysis, and tools for creating knowledge and insights.

INL applies decision science and analysis capability to meet decision-making challenges. One example is the new Laboratory Directed Research and Development (LDRD) research into methodologies for electrical utilities to prioritize protective actions against the evolution of threats from coordinated, sophisticated cyberattacks.

INL has a deep history in the development of probabilistic risk assessment (PRA) methods and tools (including nationally recognized computer models). It has unique experience in their application to evaluate complex nuclear systems for commercial nuclear power, space, and defense. The NRC’s risk-informed regulatory framework is based, in part, on insights derived from PRA. INL developed risk-informed plant safety performance measures, risk models used in the reactor-oversight process, and the internationally recognized SAPHIRE code for risk evaluation were developed by INL. INL’s PRA professionals, focused on nuclear power plant risk and safety, are likely the largest such group in the DOE complex. Complementary capabilities in plant operating data analysis and human reliability analysis round out INL competencies.

INL has also leveraged its extensive risk-assessment history in the homeland security mission space. This includes developing a risk-management framework to help evaluate all hazard risks across lifeline sectors, including their cyber and physical linkages and infrastructure dependencies and interdependencies. This involves a multidisciplinary team with highly technical skills in infrastructure analysis and applying decision science and analysis rigor in developing homeland security solutions. It includes leveraging advanced computer-science research in big data and data analytics, and visualization—especially in geospatial analyses due to the complexity and vast land areas supporting critical infrastructure. Collectively, this work helps stakeholders make better risk-informed decisions. This risk-management framework assists federal, state, and local governments, along with private sector infrastructure owners and operators, to provide a better understanding of vulnerabilities and threats and how to best mitigate and prioritize resources.

Software upgrades consistent with mission needs are further discussed in Section 4. Investments are needed to maintain the existing capabilities (including intellectual resources) at the state-of-the-art level in this quickly evolving field.
With over 110 highly trained professionals, INL applies organized, interdisciplinary approaches to solve a variety of operational, organizational, programmatic, and research problems across its facilities. INL’s leadership in this core capability is a result of an emphasis on integrating expertise across the multiple technical and operational disciplines necessary to provide reliable, quality products, processes, and services specifically targeted at helping organizations make informed decisions. INL provides the understanding necessary to help make logical, defensible, data-driven, and risk-informed decisions.

This capability aligns with both DOE and DHS missions that support nuclear energy (particularly those involved with risk and safety assessment, as well as deployment); energy security; and national security. Funding to support this core capability comes from DOE (NE, EERE, NNSA, and the Office of Intelligence and Counterintelligence); NRC; DHS; DoD; the Transportation Security Administration; NASA; EPRI; and other federal and international programs.

9. Environmental Subsurface Science

INL has capabilities in environmental subsurface science that are complemented by its chemical and molecular science and nuclear and radiochemistry disciplines. Research experience includes fundamental studies at the molecular scale to full application at industry scale. INL has developed new technologies and processes for environmental fate and transport of radionuclides, geothermal energy production, geological storage of nuclear waste, and combined recovery of unconventional fossil fuels and CO2 sequestration from nanoporous shale.

INL has demonstrated experience in integrating fundamental science into a unifying, predictive, computational framework that enables end-use application through projects such as the development of a conceptual model of contaminant distribution and transport in the deep-fractured vadose zone at the INL Site. Projects in this area employed adaptive monitoring of molecular and nanoscale processes and property changes in complex environments, resulting in predictive understanding of coupling between (bio)geochemical processes and material-property changes across spatial and temporal scales and producing computational frameworks and interoperable models for linking the subsurface environment and terrestrial ecosystems.

INL’s environmental subsurface science research is focused primarily on developing predictive understanding of: (1) the fate and transport of metal and radionuclide contaminants under natural and far-from-equilibrium conditions; (2) the geomechanical responses of the subsurface associated with extraction of energy resources (e.g., fossil and geothermal energy) and waste storage; (3) greater utilization of subsurface resources (e.g., water, minerals, and thermal energy) to support increased clean energy development; and (4) chemical and biological sensing.

This capability is supported by approximately 140 researchers and technical staff with expertise in hydrology, geochemistry, environmental microbiology, molecular biology, materials science, analytical chemistry, chemical engineering, and computational science. Close integration of these multiple disciplines is a hallmark of INL. The Laboratory has a long history of collaborations between microbiologists, molecular biologists, and geochemists as well as molecular spectroscopists, analytical chemists, and instrument builders to (1) detect and characterize environmental contaminants at the mono-layer and (2) study geomicrobiology and microbial interactions with metals and radionuclides. In addition, multidisciplinary INL research teams are recognized for conducting intermediate-scale experiments in reactive transport with mineral precipitation in porous media, integrated with reactive-transport modeling from the pore to continuum scales, as well as geophysical sensing of the evolving biogeochemistry. The studies have contributed significantly to a fundamental understanding of the coupling and feedbacks between transport, mixing, and propagation of biogeochemical reaction fronts in heterogeneous porous media.
A distinctive INL strength is the physics of multiphase flow dynamics in the deep-fractured vadose zone. INL’s commitment to this topic is derived from its unique hydrogeologic setting atop thick (varies from approximately 100 to 2,000 feet), fractured, variably saturated basalt. This hydrogeologic setting is characterized by abnormally rapid downward migration of water and contaminants over a large vertical distance for models that have been built on the conventional flow and transport theory of unsaturated porous media fail.

Over the last two decades, funded mostly through EM and SC, INL has led multilaboratory teams in a large number of unsaturated fracture flow tests of increasing scale and complexity, ranging from Hele-Shaw cells of ~1 cm size, to bench-scale (approximately 1 m) simplified analog fracture experiments, to field-scale 100-meter-diameter infiltration tests. INL also led the development of a suite of unique physics-based flow and reactive-transport codes for predicting multiphase fluid dynamics in fractures and fracture networks. The close integration of experimental and modeling studies has significantly advanced fundamental understanding of how gravitational, viscous, inertial, and capillary forces and fluid-fluid-solid contact-line dynamics interact with fracture intersections and low-permeability sedimentary inclusions. Such interactions in a deep fractured vadose zone lead to highly nonlinear—even chaotic—multiphase flow dynamics, including features such as flow focusing, spontaneous flow-path switching and episodic flow, avalanching, and cascading.

This capability is supported by state-of-the-art laboratories for materials characterization and preparation, flow and transport experiments, and chemical and elemental analysis (including isotopic analysis). In keeping with its primary nuclear energy mission, INL also maintains extensive radiochemistry laboratories and irradiation facilities. Unique within the DOE complex, INL operates a 2-m-radius geocentrifuge with a 50-g/ton capacity. The ability to conduct geocentrifuge experiments instrumented with direct (e.g., moisture sensors, pressure transducers) and indirect (e.g., miniaturized electrical-resistivity tomography) flow-monitoring devices enables rapid, unsaturated flow and transport experiments with real-world scaling. INL offers myriad locations and options for field studies (e.g., Vadose Zone Research Park) and possesses the expertise and equipment needed for extended field mobilizations.

INL recognizes that subsurface energy resources are critical to the nation’s low-carbon and secure energy future. Funded primarily by the GTO, industry, and LDRD funds, INL has developed physics-based multiscale and multiphysics geomechanical models for better predictive understanding, across all relevant scales, of changes in stress and strain fields, fracture nucleation, propagation, and coalescence in complex heterogeneous media, as well as reactivations of natural fractures and faults because of thermal, hydraulic, and mechanical perturbations. These phenomena are associated with applications such as recovery of unconventional fossil fuels from shale, engineered geothermal systems, CO2 injection, and geologic disposal of nuclear and other wastes. INL’s environmental subsurface team is positioned at the frontier of understanding the physics of fracturing stressed heterogeneous rocks, the fundamental thermodynamic laws that drive the complex and often self-organized, hierarchical patterns of fracturing; nonlinear interactions among propagating fractures and between heterogeneities ranging from mineral grains to natural fractures and faults; causal mechanisms of induced seismicity; and fracturing-energy release because of fluid injection.

INL recently finalized a contract with the Chinese High-level Nuclear Waste Disposal Program to allow INL scientists to host, mentor, and guide visiting scientists to develop hydrogeological and radionuclide-transport models near the Chinese waste-repository site. Other strategic partnerships include regional collaborations with CAES partners, other national laboratories (e.g., Lawrence Berkeley National Laboratory, Oak Ridge National Laboratory [ORNL], Pacific Northwest National Laboratory [PNNL], and Argonne National Laboratory [ANL]) and other DOE programs (Critical Materials Institute) and offices (e.g., Subsurface Technology and Engineering Research, Development, and Demonstration Crosscut;
There is a growing need within the nation to address large-scale environmental issues, including protection from potential chemical and biological threats. The ability to detect and characterize biological and chemical contaminants (e.g., industrial chemicals, toxic metals in drinking water, or chemical agents in an airport) at low concentrations is a priority to counter both deliberate acts and unintentional environmental contamination. Capabilities that enable INL’s response include analytical chemistry, microbiology, and chemical and radiation measurements. Additionally, INL has the ability to use expertise in systems engineering to demonstrate and validate new approaches using unique facilities such as the Water Security Test Bed. The goal is to provide improved response times for responders and enhanced methods for rapid screening, detection, and hazard mitigation. Additionally, INL seeks to fill critical capability gaps that would provide decision makers with needed data and options to improve resiliency, optimize responses, improve remediation, and minimize losses.

This capability has been developed through programs in the DOE’s Office of Biological and Environmental Research, Office of Environmental Management (groundwater and soil and nuclear-materials disposition), Office of Fossil Energy (carbon sequestration), EERE (geothermal technologies), and the DoD Air Force Center for Engineering and the Environment. This capability advances DOE’s missions in scientific discovery and innovation and environmental cleanup, as articulated in the DOE Strategic Plan.

10. Large-Scale User Facilities/Advanced Instrumentation

INL embraces a user facility approach to manage scientific facilities and make the capability available to researchers and industries across the Nation. The Nuclear Science User Facilities (NSUF) program is INL’s primary avenue for users seeking access to its world-class nuclear facilities. Researchers gain access (at no cost to themselves) to nuclear research capabilities (including advanced state-of-the-art instrumentation), technical expertise from experienced scientists and engineers, and assistance with experiment design, fabrication, analyses, and examination. Access is awarded through a competitive peer-reviewed process.

Over its 890-square-mile site, INL maintains a robust testing and demonstration capacity unmatched in the United States. The facilities at INL have advanced nuclear energy for over sixty years. During that time, more than 50 reactors (mostly first-of-their-kind) have been designed and built, and a comprehensive suite of allied facilities has been strategically developed across INL’s three primary research campuses. These campuses include the Advanced Test Reactor (ATR) Complex, the nation’s premier resource for fuels and materials irradiation testing; the Materials and Fuels Complex (MFC), the center of DOE’s advanced nuclear fuel development initiatives, post-irradiation examination capabilities, and transient test capabilities; and the Research and Education Campus (REC), the front door to INL and center of INL’s computing facilities, with a variety of research, administrative, educational, and technical support facilities. CAES, located at REC, is a facility collaboratively managed by INL and regional universities. It hosts the Microscopy and Characterization Suite and serves as headquarters for NSUF. These three primary areas house over two dozen discrete laboratories, hot cells, assembly facilities, and other structures, offering an unmatched set of capabilities.

As the nation’s leading nuclear energy laboratory, INL provides a broad range of capabilities, including many that are crosscutting. INL nuclear energy RD&D capabilities can be grouped into the following primary areas: fuels and materials fabrication, neutron irradiation, transient testing, pre-irradiation characterization, post-irradiation examination, separations and waste form development, reactor safety analysis, modeling and simulation, and space and security power systems.
INL also offers leading-edge facilities for non-nuclear research. National and Homeland Security programs rely on the Wireless Test Bed, which previously included the INL Wireless Test Bed; the National Security Test Range for full-scale explosives and ballistic testing of physical security technologies and armor material and system R&D and demonstration; the National Electric Research, Test, and Evaluation Grid for evaluation of threats and protective technology solutions against natural, environmental, and man-made threats; the Radiological Response Test Range for emergency response experimentation, training, and exercises; and the Water Security Test Bed for evaluation of water supply consequences as a result of chemical, biological, or cyber-attack. Additionally, the Biomass Feedstock National User Facility (BFNUF) offers technology and expertise to help the U.S. bioenergy industry overcome biomass challenges during scale-up and integration of biomass preprocessing facilities.

INL facilities are utilized by leading researchers from universities, industries, national and international laboratories, and other research organizations. For non-DOE researchers, access to INL’s facilities may be obtained through a Strategic Partnership Project, as well as through the NSUF solicitation process. User facility capability upgrades consistent with mission needs are further discussed in Section 4. Investments are needed to maintain the existing capabilities (including intellectual resources) at the state-of-the-art level consistent with the demands of the facility users.

With over 870 staff, including two joint appointments and 11 postdocs, INL provides leadership and expertise in large-scale user facilities and advanced instrumentation across the three campuses previously described.

Through its large-scale user facilities and advanced instrumentation programs, INL supports many DOE and DHS missions, with heavy focus on nuclear energy, as well as national and homeland security. Funding for this core capability comes from private and federal programs, including DOE-NE, NR, DoD, NNSA, DHS, FBI, EPRI, NRC, EPA, Crocker Nuclear Laboratory, and the Drug Enforcement Administration.

11. Mechanical Design and Engineering

INL maintains mechanical design and engineering capabilities for nuclear-system design, other energy and industrial processes, and development of technologies for evaluations of materials behavior in support of national security programs. Advanced materials and fabrication knowledge combine under this capability to achieve complex design solutions that perform reliably under extreme conditions.

This capability is founded on INL’s fundamental and applied engineering research, which provide a solid expertise base for engineering highly complex systems. The capability is applied to design, develop, test, and demonstrate components, systems, and subsystems, extending to plant-scale prototypes. The design and engineering of products include many diverse individual capabilities beyond classical mechanical engineering, to include modeling and simulation; sensing and controls; neutronic, structural, thermal, and hydraulic analysis and design; static, kinematic, and dynamic analysis; and extensive experimental prototyping and validation. INL conducts mechanical-design and engineering work to applicable standards, codes, and regulatory requirements and produces unique, innovative work in support of research requirements where standards, codes, and regulatory requirements do not yet exist.

INL is defined by its world-leading ability to build and test first-of-its-kind systems from bench to pilot and engineering scales, leading up to full-scale prototype development, demonstration, and product manufacturing. Many of the more than 50 reactors built at INL represented new designs to experimentally demonstrate the operating safety envelope for deployment purposes. Engineered prototypes include reactor and fuel-cycle facilities, as well as components to move and convert energy, robotics for remote material handling, detectors and sensors, instrumentation and controls, computer codes to predict behavior, and material and system engineering and manufacturing processes and
production lines for armor and critical infrastructure protection applications. INL utilizes its capabilities in mechanical design and engineering to support design of new energy-related projects; to develop innovative and novel solutions for warfighters to maintain U.S. battlefield superiority; to analyze, design, test, and validate unmanned vehicles; to develop advanced transportation; to drive renewable energy transmission; and to develop and use modern computational tools for engineering design and analysis.

More than 149 engineers and scientists and two postdocs support the mechanical design and engineering capability. Expertise includes mechanical, electrical, systems, and materials engineering; computer-aided design and manufacturing drafting; machining; and highly experienced technician support. Infrastructure for designing, building, testing, and validating includes the INL Research Center and associated laboratories in REC and INL personnel at CAES, ATR, MFC, SMC, and the National Security Test Range. These facilities hold general purpose engineering-scale prototype facilities, chemical and radiological laboratories, materials-development and research laboratories, HPC and simulators, and explosives and ballistic testing.

INL continues to build leadership in: (1) advanced neutronic/thermal/structural design and analysis; (2) design of complex processes, systems, and hardware for investigating in-reactor material and fuel performance; (3) microgrid support and analysis with renewable energy generation and penetration; (4) advanced manufacturing system design and process optimization; (5) performance testing and verification/validation for components and systems at scale; and (6) advanced armor applications, energetic-material development, and explosives testing.

Facility upgrades consistent with mission needs are further discussed in Section 4. Investments are needed to maintain the existing capabilities (including intellectual resources) at the state-of-the-art level in this quickly evolving field.

This capability supports DOE and DHS missions, including design, development, testing, and demonstration of nuclear energy and other energy solutions, as well as national security efforts. Funding for this core capability comes from DOE (NE, EERE, OE, and NNSA); DoD; the NRC; and industrial entities like EPRI, TerraPower, European Grup de Recerca en Radiacions Ionitzants, and KAERI.

12. Nuclear and Radiochemistry

INL has a long history and deep expertise in the unique chemistry and analysis of radioactive materials. Predicting the effects of radioactive decay and transmutation on chemical and material behavior in applications such as energy production, waste management, and nuclear nonproliferation is an essential part of INL’s mission. INL has extensive research and operations experience with nuclear and radiochemical separations technologies at bench and engineering scales. In the 1980s, INL built and operated the only U.S. second-generation aqueous reprocessing facility, where it developed broad experience in nuclear and radiochemical separations on spent nuclear fuel types, including aluminum, zirconium, stainless steel, and graphite fuel. INL designed, built, and operates the only engineering-scale electrochemical separations R&D facility in the U.S. The Laboratory’s access to used fuel, combined with expertise and facilities for used-fuel handling, affords unique capabilities in all aspects of radiochemistry.

INL’s expertise in solvent extraction and radiochemistry allows lead leading research in nuclear and radiochemical separations technology. Today, INL scientists and engineers apply this expertise to address challenges in two areas. First, they support clean energy by vastly improving fuel-cycle separations for mitigating nuclear waste issues. They also develop predictive and manipulative capabilities for safer, more efficient handling of radioactive material. Second, they improve national security by advancing nuclear forensics, reducing the stockpile of nuclear material, and producing isotopic-trace-measurement standards.
The radiochemistry laboratories support experimentation with actinide and activation product elements. Experiments on the effects of high-radiation fields on the properties of solutions and solid materials are conducted using irradiation facilities at INL (radiation test loop and NSUF). Measurement of trace levels of radioisotopes in environmental matrices using clean-room sample preparation and specialty mass spectrometry, including an accelerator mass spectrometer and mass separators, allows rapid detection of extremely low concentrations of rare isotopes. Another INL research focus is the evolution of matrix chemistry during continued radiolysis which is evaluated by measuring transient radical and ionic species in solution and the gas phase. These experiments are important for monitoring nuclear-waste separations and storage and for predicting the performance of long-term containment measures.

INL provides leadership in radiochemistry relative to solvent-extraction technologies and free-radical chemistry, thermodynamics and kinetics of liquid-liquid extraction process chemistry, solvent-extraction process chemistry, nuclear nonproliferation verification, and nuclear forensics. These applications leverage capabilities in chemical and materials sciences; irradiation services in ATR for plutonium-238 isotope production; and radiation measurement science. Key distinguishing activities supporting nuclear-forensics radiochemistry at INL include the use of electromagnetic isotope separation instruments for stable and radioactive isotope enrichment and the use accelerator-based photofission and photonuclear reactions for production of radioisotopic and stable-isotope standards for mass spectrometry. Word-class mass spectrometric measurement and instrument design expertise complement these capabilities.

Facility upgrades consistent with mission needs are further discussed in Section 4. Investments are needed to maintain the existing capabilities (including intellectual resources) at the state-of-the-art level as this is a critical capability in which U.S. leadership is rapidly eroding.

Approximately 116 experts, including one joint appointment and three postdocs, support the nuclear and radiochemistry capability. Extensive Laboratory infrastructure in support of this capability includes the Analytical Laboratory, Radiochemistry Laboratory, Fuels and Applied Science Building radiolysis/hydrolysis test loop and gamma irradiator, EIL, Fuel Manufacturing Facility, and ATR. In addition, INL has extensive university and international collaborations that leverage available academic capabilities while helping to prepare a new generation of radiochemists.

DOE and DHS missions that INL furthers through this core capability include optimization of nuclear energy systems (particularly in consideration of energy and waste generation), national security, and environmental management. Major funding for nuclear and radiochemistry at INL comes from DOE (NE, NNSA, and SC), NASA, and other agencies within DoD and DHS.

13. Nuclear Engineering

Nuclear engineering is a core capability and key area of expertise at INL. This capability is founded on its historical role as the National Reactor Test Station, which built, operated, and tested more than 50 reactor prototypes, in addition to hosting many large-scale reactor safety experiments. Similar activities are ongoing today as the Laboratory supports the primary mission of DOE-NE through nuclear systems design, operation, and safety analysis; advanced fuel material development and testing; high-temperature chemical and electrochemical separations; engineering-scale pyroprocessing treatment facilities; radioisotope power system fueling, testing, transport, and ground operations; technical and policy support for nuclear regulatory agencies; study of economic and market factors affecting nuclear energy systems; hybrid energy systems; nuclear nonproliferation and international safeguards; nuclear counterproliferation; nuclear forensics; nuclear cybersecurity; emergency response technology and training; global threat reduction through conversion of highly enriched uranium (HEU) fuels to low-enriched uranium (LEU); and nuclear systems performance M&S.
INL’s nuclear engineering expertise draws upon multiple disciplines required to analyze, design, demonstrate, deploy, and operate nuclear systems. These include capabilities in neutronics, thermal hydraulics, structural-design analyses for small- and large-scale experiments, mechanistic and probabilistic safety and other risk analyses, development of robust materials for the nuclear environment, and development of destructive and nondestructive nuclear materials detection and safeguards technologies. Interdisciplinary teams apply expertise in critical infrastructure protection, robotics, cybersecurity, electric power grid resilience, and physical protection to resolve broad challenges that impact national and international nuclear security.

INL has substantial experience with the application of modern software to perform integrated neutronics, thermal-hydraulics, and structural analyses for nuclear systems for the commercial nuclear power industry and defense, space, and regulatory communities. It also has decades of leadership in the development of reactor safety analysis codes by sustaining the Reactor Excursion and Leak Analysis Program (RELAP) code series. INL researchers work on the next generation of reactor safety codes by incorporating state-of-the-art software engineering and two-phase flow solution algorithms. INL also has an extensive history in the development and use of PRA, including the leading codes that are in use today (see subsections 3.1 and 3.8). In addition, INL nuclear engineers support the safe and reliable operation of ATR, ATR Critical Facility, NRAD, and TREAT. Nuclear engineering work is also underway at INL to design, prototype, and test research-reactor fuels for reactor conversion from HEU to LEU, and to develop state-of-the-art instrumentation and control systems to enable better experimental digital control, wireless communication, and data acquisition.

INL’s nuclear engineering assets evaluate the proliferation risks of advanced fuel-cycle input and associated material streams. INL uses this information to improve safeguards approaches and instrumentation to address vulnerabilities and enable the U.S. to support global initiatives for the deployment of nuclear energy and the recovery, transport, and secure storage of nuclear and radiologic research materials.

Facility upgrades consistent with mission needs are further discussed in Section 4. Investments are needed to maintain the existing capabilities (including intellectual resources) at the state-of-the-art level as this is the kernel for the primary mission of INL.

Approximately 448 technical experts, including three joint appointments and 11 postdocs, are dedicated to INL’s nuclear engineering efforts. Laboratory infrastructure supporting these activities includes the Space and Security Power Systems Facility at MFC; the Fuel Conditioning Facility; TREAT; ATR and ATR Critical Facility; NRAD; and HFEE capabilities. MFC is the only location in the world with an engineering-scale, operational, and remotely operated pyroprocessing equipment in an inert hot cell.

Funding for this capability comes from DOE (NE, SC, NR, and NNSA) other agencies such as NASA and DoD and industrial entities including EPRI, KJRR, EDF Energy, Westinghouse, NuScale, TerraPower, and Babcock and Wilcox.

14. Power Systems and Electrical Engineering

INL’s power and electrical-engineering team’s scientific experts, together with leading power engineers with industry experience, conduct RD&D using the nation’s largest high-power and evaluation test range, a facility consisting of a microgrid and a digital real-time simulator (DRTS). DRTS is located in the ESL and operated under the National and Homeland Security programs. The DRTS is configured for hardware-in-the-loop (HIL) experimentation and advanced scientific research by interconnecting electric vehicles at the Electric Vehicle Infrastructure Laboratory (EVIL), the microgrid, and thermal-energy devices as they become available. The DRTS facility offers advanced modeling, simulation, and testing capabilities where electric-power systems, fast-switching power electronics, and communication for acquisition and controls can be simultaneously simulated in real time. The INL DRTS is currently
associated with multiple DOE and DoD programs, ranging from the electrical-power, transportation, and industrial-manufacturing sectors to wireless communication systems and to infrastructure for unmanned aerial vehicles operating at the INL Site. It also supports industrial needs in the utility sector and manufacturers of power electronics equipment.

INL’s DRTS is a one-of-a-kind research infrastructure and the largest setup of DRTS assets in the DOE laboratory complex. DRTS provides both high-fidelity simulation of power systems and HIL emulation for fast, reliable, accurate, and cost-effective study of power systems, power electronics, thermal systems, and controller-communications protocols. It is an electromagnetic-transient program-based power-system simulator that operates in real time, allowing the user to test physical devices (i.e., power HIL, grid-in-the-loop, and controller HIL). DRTS also permits assessment of power-flow management, both to and from critical energy systems. As part of the research using DRTS, an LDRD project demonstrated the proof-of-principle that the capability exists to successfully interconnect and synchronize with a DRTS at National Renewable Energy Laboratory. Engagement with universities, utilities, and research organizations in the region has culminated in additional research projects.

INL leads research in hybrid energy systems design, analysis, and HIL testing; state-awareness diagnostics, prognostics, and control-data analysis; process-system state analysis; mitigation of damaging effects of natural and man-made hazards, including geomagnetic disturbance and electromagnetic pulse; DoD energy system applications; electrical- and economic-modeling analysis; and performance design-requirements development. The unique combination of resources, including a real-time, high-fidelity physics-based power and radiofrequency M&S, allows INL to deliver advanced energy-systems security research and testing. Design, integration, and evaluation expertise are combined to realize dynamic systemwide energy solutions to optimize power and thermal control, stability, reliability, communications and security.

INL’s campus and Site boundaries provide access to isolated, secure, industrial-scale facilities and infrastructure for conducting comprehensive interoperability, vulnerability, and risk-assessment activities. These assets include (1) the National Electric Research, Test, and Evaluation Grid, which includes an isolatable and customizable utility-scale 138 kV transmission system and 13.8 kV, 15 kV, 25 kV, and 35 kV class distribution voltages with multiple concurrent test areas; (2) the Microgrid Test Bed; (3) CITRC; (4) the Wireless Test Bed; (5) the Energy Storage Test Laboratory, (6) the DRTS; (7) the Human Systems Simulation Laboratory, and (8) the Control System and Cybersecurity Innovation Laboratories. These capabilities, unique in terms of physical infrastructure, can be configured and utilized for cutting-edge research by interconnecting these systems. Because DRTS provides the interfacing capability for actual power hardware and controls, it resides at the center of the advanced power and energy-systems research. INL’s power grid operates under a full range of climatic conditions (e.g., temperature, wind, snow, ice). With the highly instrumented grid, INL can safely isolate grid sections and associated testing infrastructure to conduct full-scale testing and validation of technology components, security and resilience, systems, and processes. Industry can use this capability to test owner-specific equipment, even to the point of system failure, and utilize DRTS for large-scale testing under realistic scenarios.

INL’s holistic approach to resilient energy systems integrates cyber and physical security with efficiency and stability as performance constraints to optimize power-system operations and mitigate threats. By developing and maintaining robust, full-scale cyber- and physical-security analytics capabilities, INL ensures that legacy and modern industrial control systems have the best available defenses to protect energy-systems operations. With an eye toward the next generation of control architectures, INL conducts interdisciplinary instrumentation, control, and intelligent-systems research to enhance the resiliency of energy systems. INL’s power and electrical-engineering staff and capabilities also support work for others in the area of energy assurance and power-systems reliability for the DoD, DOE, industry, and academia. This includes assessments of fixed installations and mobile systems to ensure an
 uninterruptable supply of electricity under various situations and smart-technology development for increasing installation and operational energy efficiency. DRTS plays an important role in enabling the co-simulation of several infrastructures from a real-time cyber-physical perspective at a very fast rate.

ESL provides DRTS-enabled experimental infrastructure with a capability for integrated testing of a microgrid and future thermal-energy-systems engineering in a high-fidelity real-time environment. INL focuses on system-level applied engineering to allow industry and government to optimize nuclear energy in HESs through grid integration of electric power and thermal energy while addressing technical issues, such as intermittent, variable generation and energy storage. The microgrid-research laboratory component testing and systems integration represents current and evolving power-generation systems that require flexible operation of larger nuclear thermal energy generation plants.

In addition, the DRTS capability supports development of power electronic and controller hardware, protection devices, EV-charging infrastructure, renewable-power-generation test units, and electrical flow battery. It will include a thermal-energy-storage and recovery system, an emulated nuclear thermal-energy generation and delivery loop, and industrial process-heat-application station. DRTS is connected to the EVIL hardware and is configured for integrated testing using actual grid interfaces though a hardware grid emulator. This capability provides solutions for newer technologies, nondispatchable electricity production and delivery onto the grid, flow control into and through the grid, and optimized energy-storage size and location in the electrical supply chain. The fundamental concepts of such systems-level capabilities are also applied to other domains to secure energy assurance and power reliability for critical infrastructure, including fixed installations, mobile military systems, vehicles and advanced transportation systems, and other pulsed power systems.

The core power grid used for INL’s full-scale testing and evaluation is primarily used to power INL Site operational facilities. Therefore, the grid is supported under operational funding from NE. Specific test configurations are funded directly by the projects under test and evaluation at INL, including projects for DOE, DHS, DoD, California Energy Systems for the 21st Century, and other government, private, and industrial agencies. More than 50 technical experts bring together expertise in power, control systems, and engineering. The end users are the ultimate customers for these capabilities, as are the RD&D customers such as NE, OE, NNSA, and EERE.

15. Systems Engineering and Integration

INL is a recognized leader in solving problems holistically—by synthesizing multiple disciplines to develop and implement optimal solutions—from concept and design to the ultimate deliverable and completion phase. INL leverages its legacy competency in conceptualization, design, operation, and analysis of prototypic complex systems to assist regional and national:

- Industry to reduce the time and cost of energy- and security-technology deployment
- Regulatory agencies to set appropriate standards by providing science-based data
- Policymakers to establish the viability of advanced technologies.

This capability base incorporates the other INL core-capability components, grounded in INL’s historical roots, sets INL apart as a distinctive national laboratory.

INL’s mission objectives promote the evolution of innovative regional partnerships that employ regional assets, teams, and capital to achieve regional leadership in clean energy innovation. To assist the DoD in meeting aggressive renewable-energy portfolio mandates nationally and regionally, INL performed economic and business-case analyses for a potential wind project at Malmstrom AFB and the Air National Guard in Great Falls, Montana. Also, INL has partnered with the Wyoming Resources Institute to perform technical and economical assessments for their efforts to establish synfuel/hydrogen
production by converting a process feed of at least 50 percent coal into higher-value products. In addition, a nuclear hybrid energy-system feasibility study was completed for the state of Wyoming.

Responding to national needs over the last 60 years, INL has built substantial capability for understanding, designing, prototyping, optimizing, and operating complex systems. Examples include prototype hybrid-renewable and clean energy systems, advanced nuclear reactors and reprocessing facilities, waste- and SNF-management pilot facilities, advanced vehicle and battery testing and analyses, industrial and DoD cybersecurity, and protection for electrical transmission systems. INL’s newly established Dynamic Energy Transport and Integration Laboratory (or DETAIL) offers a unique capability to assess the complexity of nuclear/fossil/renewable hybrid energy systems that convert, transport, and use energy currency provided by these resources. This capability includes a microgrid with renewable power generation, thermal-energy storage, power consumption via vehicle charging stations, and a digital real-time simulator that emulates power-generation sources and the electric grid.

Expertise initially developed to characterize the viability, safety, and operational characteristics of nuclear-reactor designs are still in operation today. This includes capacity to characterize associated energy-conversion and control technologies. These have expanded to the development, design, and deployment of fuel-cycle technologies, hybrid energy systems, resilient design, and recovery of critical infrastructure; consequence-driven cyber-informed engineering integrating high-fidelity physics-based modeling, full-scale experiments, the most instrumented industry-scale test grid; and testing of related components, subsystems, and systems that play a critical role in national security.

INL retains systems-engineering capabilities that support design and fabrication activities, experiment design and development, instrumentation controls, data analyses, and quality assurance. These capabilities comprise a strong combination of research engineering and operational skills, distinctive experimental infrastructure, and educational partnerships. Other examples of systems engineering and integration that resulted in the development of testing and demonstration capabilities are the PDU for industrial-scale preprocessing of biomass feedstocks into commodity-grade standardized fuel pellets and a full-scale prototype waste-package system for repository use. Each deployed teams of engineers and scientists assembled from across the Laboratory to solve a complex engineering problem.

INL systems expertise helps ensure that the modern smart grid incorporates secure smart communications and distributed generation resilience against geomagnetic storms, electromagnetic disturbances, and cyber or physical attacks with interdependent, cascading consequences. An extensive Laboratory infrastructure supporting these activities includes the laboratories and facilities previously mentioned and a wide range of general-purpose engineering-scale prototypes, chemical and radiological laboratories, materials-development, grid, and research laboratories. This expertise and these physical capabilities are increasingly deployed as national user facilities, through which industry, government, and academic researchers can engage INL staff to carry out research, development, integration, testing, and demonstration.

Approximately 250 technical experts, including one joint appointment, combine expertise in systems engineering and integration to conduct problem identification and management of technical, functional, and operational requirements and project risks. These experts identify viable technology alternatives and conduct R&D to mature them; they select and implement optimal and defensible solutions for energy, environment, and security systems. Trained experts have graduate degrees, certifications, and significant experience in the application of systems engineering as defined in national and international standards on complex nuclear, national and homeland security, and energy and environmental systems.

The INL’s systems-engineering and integration capabilities are applied to programs of regional, national and international importance, including those for NE, EERE, OE, and NNSA; other agencies such as DoD, DHS, and the Drug Enforcement Administration; and industrial entities such as NuScale, TerraPower, and...
EDF Energy. These capabilities are also the basis of U.S. technical engagement with other countries (e.g., United Kingdom Nuclear Decommissioning Agency).

Science Strategy for the Future

INL’s S&T strategic initiatives help achieve the critical outcomes listed in Table 4.1. They are designed to advance scientific and technological capabilities and sustain and build INL’s core capabilities and leadership positions to provide for national scale energy and security solutions for DOE in critical mission areas. As an applied-energy laboratory with unique geography, INL retains core competencies and capabilities to develop, test, and demonstrate advanced concepts for proof of concept and technical and economic viability.

INL’s nuclear energy related initiatives focus on building, demonstrating, and deploying capabilities and creating partnerships, both domestically and internationally, in nuclear research. INL will build upon its national and global leadership in nuclear energy RD&D and develop effective and integrated spent nuclear fuel cycle solutions for management and disposition of SNF and high-level nuclear waste to support projected nuclear energy demand. Leveraging these capabilities, INL will build expanded understanding and develop and deliver nuclear energy and integrated spent nuclear fuel cycle solutions to address challenges that will:

- Enable advanced nuclear energy systems through public/private partnerships
- Build innovative experimental capabilities, including a fast-spectrum reactor
- Develop and demonstrate advanced nuclear and small modular reactors
- Design and develop advanced materials and fuels for advanced reactors
- Develop solutions for integrated management and disposition of nuclear waste
- Build advanced M&S tools and integrating them with experimental capabilities to accelerate development and deployment of nuclear technologies.

Leaveraging INL’s recognized leadership and capabilities in solving problems holistically, INL will focus on accelerating the pace of energy and environment-technology innovation and transition using regional partnership and deployment. INL will close the gap between supply and demand, address technology-deployment challenges by designing and developing hybrid energy-system solutions that couple nuclear-, renewable-, and fossil-energy sources with the grid to optimize energy use for combined electricity, transportation, and industrial-sector applications. INL will mitigate risk in the design and operation of nuclear energy systems through innovations in advanced manufacturing capabilities for designing and developing smart materials for harsh or demanding environments and optimized chemical, material, and energy processes that convert strategic materials and waste into energy and products, conserve energy, and limit hazardous emissions and residuals.

As a globally recognized R&D leader in nonproliferation technologies, nuclear safeguards, critical infrastructure protection and control systems cybersecurity, INL will make important technology advancements to secure and modernize the nation’s critical infrastructure, emphasizing the protection

Table 4-1. INL’s Critical Outcomes

| 1. | Build nuclear energy competitiveness and leadership |
| 2. | Develop integrated spent nuclear fuel cycle solutions |
| 3. | Develop advanced hybrid energy systems |
| 4. | Establish enduring cyber-physical innovation capability centered on Cybercore Integration Center to advance cyber-informed science and engineering |
of energy, nuclear, and military systems. A strategic component in achieving this vision involves the development and implementation of the Cybercore Integration Center. The Cybercore Integration Center vision is to realize a future blending of cyber, physical, and behavioral sciences with new engineering methods to design, build, and operate secure systems, processes, and infrastructure. A foundational principle of Cybercore Integration Center is to effectively enable digital, wireless, and autonomy technologies, while simultaneously addressing security during the design phases of next generation network architectures and communications.

Strategic partnership and collaboration nationally and internationally are key elements in executing INL’s mission to achieve its strategic objectives. INL will continue to build partnerships with other national laboratories, universities, and industry to support mission objectives and advance capabilities, accelerate innovation, support demonstrations, accelerate deployment of technology advances, pool capabilities and resources, and enhance INL’s science and engineering pipeline. As capabilities expand, the Laboratory will continue to make its distinctive research facilities and expertise available to the scientific user community on a competitive basis. To facilitate mission growth, and grow partner engagement, INL will require a new footprint and specific facility attributes not achievable with the current footprint and capabilities. Facility needs and plans will be discussed in the relevant subsections below and in the infrastructure section of this plan.

INL is in the process of developing a public international strategy, taking into account recommendations of the Nuclear Energy Advisory Committee as well as building on international efforts that have not previously been defined in a public strategy. INL has been focused on S&T collaborations, primarily at the program level, with traditional partners from Europe, Japan, and Korea. New efforts began recently to develop new collaborations with emerging nontraditional nuclear energy countries, including China, India and Vietnam, where INL’s unique capabilities give the U.S. unprecedented access to developing R&D programs as well as developing safety standards and practices. INL also continues to build effective frameworks for engagement with international agencies, including the IAEA, Nuclear Energy Agency (NEA) of the Organization for Economic Cooperation and Development, the Generation IV International Forum, and the European Union, etc. INL staff are part of the technical program committee for IAEA’s international nuclear safety workshop.

INL uses discretionary resources to strengthen its core capabilities, advance the Laboratory’s mission, and achieve its strategic objectives. The annual LDRD budget is developed after careful consideration of investment needs and overall INL indirect budget. The final LDRD budget-cap request is developed and approved by INL’s Laboratory director. The LDRD program benefits INL and DOE by providing the Laboratory with resources for developing new R&D capabilities to better meet DOE’s and the nation’s needs, to seed innovative research, and to attract and retain research staff who maintain the vitality of the Laboratory. INL’s LDRD plan aligns with INL’s S&T strategy and is detailed in Appendix B.

These capabilities will be leveraged and advanced to solve complex global security challenges in the areas of critical infrastructure protection, nonproliferation, and national and homeland security. Our strategy to achieve the four critical S&T outcomes are discussed in the following subsections.

Building and growing international competitiveness and leadership will enable INL to improve innovation capabilities, collaborate more broadly, and solve more-complex problems to address energy and security challenges. To achieve these objectives, INL will raise scientific impacts of the Laboratory through improvement in INL’s S&T ecosystem and culture. Initiatives to improve time, travel, and training are currently underway. INL’s time-billing initiative will provide flexibility in reporting to support S&T staff’s mission and development activities and to help staff members balance work-life priorities. The training initiative is focused on making training courses value-added and efficient. The travel initiative will streamline processes, automate tools, and create mobile apps that provide INL staff more access, autonomy, information, and support services. Finally, INL will enhance publications-data quality
and tracking, implement an S&T dashboard, and improve the quality, relevance, and impact of S&T outputs, including publications and intellectual property.

Infrastructure

Overview of Site Facilities and Infrastructure

INL is located in southeastern Idaho, with assets and capabilities residing in Idaho Falls and on the INL Site (see Figure 6.1). INL’s core capabilities are consolidated around several research areas on the Site: the ATR Complex is the primary location to conduct thermal irradiation; MFC provides shielded hot cells to handle highly irradiated materials, gloveboxes to handle special nuclear material, and the TREAT facility for transient testing; CITRC primarily serves the Laboratory mission to secure critical infrastructure and safeguard nonproliferation, including critical infrastructure resilience and nonproliferation experimentation, testing, and training; SMC houses unique assets underpinning DoD missions; Idaho Nuclear Technology and Engineering Center (INTEC), currently owned and operated by EM, is home to several facilities that support INL’s spent nuclear fuel capabilities and may also support future INL customer needs; Central Facilities Area (CFA) supports the Wireless Test Bed network-operations center, the main Sitewide protection, emergency response, network and communications, transportation, and warehousing services for the Site campuses. Idaho Falls is home to Research and Education Campus, where primary focus is on nonradiological laboratory-based research to support NE: at-scale clean energy systems integration and demonstration, national security program capabilities, and Laboratory administrative functions.

INL real property infrastructure includes 534 NE owned and operated real-property assets with a total replacement value of $4.8 billion. These assets include 298 operating buildings (totaling 2.3 million gross ft2), 232 nonprogrammatic other structures and facilities, and four “programmatic” real-property assets that fall into the 3,000 series Facility Integration Management System (FIMS) other structures and facilities (OSFs) usage-code category, as well as ATR, its cooling tower and vent stack, and the TREAT. The inventory includes 24 mission-critical assets. The facilities accommodate approximately 4,300 people on a daily basis, including employees, facility users, subcontractors, and others. Sitewide utilities
and supporting infrastructure, consisting primarily of roads, railroads, power-distribution systems, and communication systems, are maintained and operated to serve and connect the campuses and facilities.

**Campus Strategy (Overall Approach to Infrastructure Sustainment)**

Four critical outcomes (see Section 4) form the basis for the Laboratory’s campus-development and infrastructure-investment and sustainment strategy. INL is on a positive infrastructure trajectory with a comprehensive approach focused on aggressive stewardship of assets to enable the Laboratory mission and achievement of critical outcomes. Informed by condition assessments, utilization studies, and integrated with comprehensive maintenance planning, INL utilizes five-year infrastructure investment plans for each of the main campuses to capture and identify gaps and establish priority investment needs.

INL’s infrastructure sustainment strategy has seven main focus areas (listed below) to revitalize or replace facilities that cannot meet the required functionality in support of INL’s mission and achievement of Laboratory’s critical outcomes:

- Leverage existing and establish new capabilities
- Sustain key campuses
- Address excess facilities
- Manage waste liabilities
- Optimize space and land use decisions
- Upgrade computing infrastructure
- Enhance Site sustainability

One or more of the seven focus areas are reflected in the planned changes and priorities to each of INL’s research campuses. The campus’ capabilities link to critical outcomes, and planned infrastructure changes to optimize achievement of Laboratory outcomes are discussed below. Near-, mid-, and long-term changes to the campuses have been envisioned in the INL Campus Master Plan and are incorporated into INL’s comprehensive campus infrastructure strategy as priority and funding allow. Summary of changes to each of the main campuses are discussed in the subsections below.

**Advanced Test Reactor Complex**

The ATR Complex houses ATR, one of the world’s most versatile materials test reactors and a mission-unique facility serving as a cornerstone supporting INL’s nuclear energy competitiveness and leadership critical outcome. A low temperature, pressurized-water cooled reactor for steady-state irradiation, ATR supports nuclear energy research and materials irradiation for DOE, EPRI, NR, KAERI, and several university and industrial collaborators through the NSUF. The ATR has operated for almost 50 years, and the facility has an indefinite lifespan because of routine, planned replacement of the entire reactor internal structure at approximate 10-year intervals. Investment needs for the remaining majority of the plant infrastructure have been defined in the ATR 5 Year Plant Health Investment Strategy Update (CCN 239988). The plan established a mission need for strategic, risk-based investments to improve ATR plant reliability to achieve predictable annual operation to meet customer needs, to address significant deferred maintenance needs, and to expand its experimental capabilities.

In addition, the need to consolidate, refurbish, and renovate general-purpose support infrastructure and for mockup and preparation space is planned to be alleviated through the addition of the ATR Maintenance and Support Building (previously known as the ATR Technical Support Building). The proposed building will need to be in place to support the planned 2020 core-internal change activities.

**Materials and Fuels Complex**

Reviving and enhancing/advancing the historical MFC capabilities to support demonstration-scale activities is imperative for INL to achieve the following critical outcomes: (1) nuclear energy
competitiveness and leadership and (2) integrated nuclear fuel cycle solutions. Need for continuing investment in the aging infrastructure is addressed in more detail in the MFC Five Year Investment strategy (INL/EXT-16-40178), a companion document to the MFC Integrated Five-Year Roadmap (INL/EXT-16-37720) that defines specific implementation strategies for increasing research capability and throughput to achieve INL critical outcomes. Planned investments support the mission to accelerate development and deployment of nuclear energy solutions through GAIN and provide access to these unique and valuable capabilities to national laboratory, industry, university, and international users through implementation of a user-facility model.

Identified gaps in transient testing are being addressed through investments to restart TREAT. Gaps in nuclear-materials characterization and examination will be addressed by building the Sample Preparation Laboratory and the MFC Research Collaboration Building. Infrastructure investments will also support development of technology solutions for safe and secure storage and disposition of the existing inventory of civilian and defense SNF and HLW.

Investment in general-purpose infrastructure, as well as consolidation and modernization of existing facilities, is needed, including innovative solutions to resolve office-space congestion. MFC priorities for collaboration and office space are increasing relative to other use needs as the population of the research campus grows and as currently obsolete modular office space, no longer suitable to support MFC, is removed.

To resolve this, additional strategy has been proposed using discretionary indirect funding to replace 10,032 ft² of leased and 31,989 ft² of old permanent modular structures and trailers at MFC that are currently providing substandard office space for researchers and scientists. The strategy includes collocating and consolidating staff into approximately 37,300 ft² of new temporary modular office buildings until permanent buildings can be constructed. The old structures will then be removed, thereby eliminating approximately 8,200 ft² of office space, and $130,000 in deferred maintenance and repair needs.

**Specific Manufacturing Capability**

SMC is the last remaining program at Test Area North (TAN) and is anticipating 10 to 15 years of continuing operations to support national homeland security missions. The need for continuing investments in TAN’s aging infrastructure is critical in keeping the SMC project going forward into the future. Documented in the SMC five-year plan for infrastructure investment, primary lifecycle issues are the TAN 601 dial room, TAN potable-water system, power-distribution system, heating, ventilation, and air conditioning (HVAC), roofs, and the roads and grounds. INL’s comprehensive investment strategy incorporates SMC’s general purpose needs in its indirect-investment strategy.

**Research and Education Campus**

REC serves as the “Gateway to INL” and provides a primary entry point for the user community to INL capabilities. In support of achieving nuclear energy competitiveness and leadership, INL has transformed REC to be more conducive for collaboration with industry and university partners while providing the latest in laboratory and office efficiencies. REC includes key research infrastructure residing in EIL and IRC and supports primary capability for advancing modeling and simulation, and includes the planned addition of Collaborative Computing Center. REC also includes capabilities to advance hybrid-energy-system integration, advanced transportation, and advanced manufacturing to accelerate the pace of impactful energy innovation. INL’s Cybercore Integration Center—which will help solve complex global security challenges in the areas of critical infrastructure, national and homeland security, nonproliferation, and intelligence—will be built at REC. Investment to update and repurpose the IRC labs is ongoing to support multiple mission outcomes.
Office-space congestion and underutilized space on the REC campus are targeted for improvement through zoning and efficiency activities, such as the establishment of several “touchdown zones” to accommodate non-resident employees and visitors at in-town facilities.

Leverage Existing and Establish New Capabilities

To build nuclear energy competitiveness and leadership and develop integrated spent nuclear fuel cycle solutions, INL is focused on expanding, revitalizing, and sustaining key DOE-NE experimental and test-bed capabilities, integrating the experimental and test-bed capabilities with advanced M&S capabilities, and increasing access of these unique capabilities to the nuclear energy community. Improvements to experimental and test-bed capabilities at MFC and ATR, enabling the next generation of high performance computing, advanced M&S, and integration with experimental capabilities in particular will reduce time to innovation and market. DOE-NE, with NR, is also constructing a replacement facility for onsite disposal of remote-handled low-level nuclear waste (RH-LLW).

To enhance capabilities in cyber-informed science and engineering INL will establish the Cybercore Integration Center to address infrastructure gaps that limit INL’s continued leadership of associated programs and R&D of critical cybersecurity solutions. Gaps include a lack of reconfigurable cyber- and electronic-research laboratory spaces (unclassified and classified), office space for researchers adjacent to laboratory areas, special development areas (at all levels of security configuration), connections to key customer information networks, and the ability to have functional connections to private customers.

![Figure 6.2. Investment overview and timeline](image-url)
Figure 6.2 provides a timeline of planned infrastructure investments and priorities that will result in robust enhanced capabilities to achieve critical outcomes and advance enabling enterprise infrastructure.

**Sustain Key Campuses**

Beyond leveraging existing and establishing new capabilities, it is imperative that the Laboratory sustain general-purpose infrastructure supporting those capabilities. Investment for sustaining key campuses is informed by the following five-year plant-health strategies:

- The Materials and Fuels Complex Integrated Five-Year Strategic Roadmap (INL/EXT-16-40178)
- The Advanced Test Reactor 5-Year Plant Health Investment Strategy Update (CCN 239988)
- The SMC Infrastructure Management Plan (SMC-PLN-211 addresses investment needs, gaps, deferred maintenance, plant-reliability improvement strategies, and footprint management)
- Five-year infrastructure plans for Sitewide utilities and Balance of Plant that are under development.

These plans maintain focus on sustaining priority, general-purpose, enabling infrastructure that underpins mission success. INL invests close to $50 million annually in needed maintenance, repair, and upgrades of general-purpose infrastructure. These investments are from a variety of funding sources, including federal appropriations for line-item construction projects, general plant projects, and plant-health investments, as well as overhead-funded investments in institutional general-plant-project work and routine maintenance and repair.

INL is also committed to providing employees and visitors with modern, collaborative, and sustainable work environments that are safe, accommodating, flexible by design, and capable of reconfiguration. To address this commitment, as new facilities are built or existing facilities upgraded, the following principles are applied to meet specific program and project needs:

- Consolidate space and co-locate support functions in renovated, modern spaces.
- Improve movement about the campuses by developing a wayfinding strategy to simplify and safeguard circulation, transportation, and pedestrian pathways and gateways on INL campuses.
- Provide safe and reliable bus transportation from local communities to INL on-site campuses at no cost to the employee through the INL transportation system, a critical component of INL safety culture.
- Optimize existing parking lots to gain capacity, enhance efficiencies in bus transportation, and develop new parking lots to meet growth and sustainability objectives.
- Emphasize environmentally sustainable practices in campus operations and processes as renovations of existing space are performed.
- Maintain the security of nuclear operations, fundamental to successful mission outcomes; DOE continues to make the necessary investments to ensure compliance with security requirements.

An added benefit of funding and execution of the infrastructure investment plans is the forecasted downward trend in deferred maintenance, as shown in Figure 6 3. Idaho Facilities Management Program investments of close to $33M in ATR and MFC in FY 2016 and in general purpose infrastructure ($23M in INL Power Distribution in FY 2016-FY 2017 and $15M in roads in FY 2017) are now showing positive impact as measured by deferred maintenance reduction starting in FY 2017.
Address Excess Facilities

In addition to infrastructure improvements, INL will continue to leverage the “Reduce the Footprint” and “Freeze the Footprint” initiatives to champion real-property stewardship practices that support the Department’s Real Property Efficiency and overall Asset Management Plans. INL identifies unneeded real-property assets excess to mission needs for reuse or disposal per federal real-property disposition requirements. It is INL’s goal to offset new construction through the elimination of equivalent excess facilities—especially for office or warehouse needs. Typical methods of elimination include demolition and lease termination or expiration.

Strategic emphasis has been on eliminating excess facilities at the CFA area. During FY 2016, INL demolished two of five historical Naval Proving Ground signature properties located at CFA. Two additional facilities were demolished in FY 2017. Demolition was performed in accordance with a signed Memorandum of Agreement between DOE-ID and the state of Idaho and after completion of a Historic American Landscape report provided to DOE-ID, the State Historical Preservation Office, U.S. National Park Service, and Advisory Council on Historical Preservation (reference INL/EXT-15-35931, INL/EXT-15-35895, and INL/EXT-15-35824).

Funding has been secured to implement the next steps of the building disposition strategy. In FY 2017, INL has initiated assessment and remediation to deactivate and demolish two additional excess contaminated buildings—the Health Physics Instrumentation Laboratory, CF-633, at 19,833 ft², and the Radiological and Environmental Sciences Laboratory, CF-690, at 32,394 ft². These buildings are listed as INL site priorities 1 and 2 in FIMS and on the DOE National Laboratory Operations Board Excess Contaminated Facilities Working Group inventory. The Health Physics Instrumentation Laboratory building is the last Naval Proving Ground building approved for demolition under the Memorandum of Agreement with the state. Following demolition of CF-633 and CF-690, focus will turn to two technical-center office buildings constructed in 1963—CF-688 at 19,312 ft², and CF-689 at 26,795 ft²—that are vacant and no longer needed for mission work.

Direction for completing excess facility decommissioning and demolition (D&D) is maintained through an active building-disposition strategy that includes a summary of estimated costs, status, hazards, and risk ranking, and estimated year of elimination. Excess assets include those with shutdown-related FIMS
status codes for buildings, trailers, and OSFs (FIMS Status Codes 3, 4, 5, 11, and 12). The actual investment and disposition square-foot profile will depend on the amount of funding that is ultimately allocated to this effort. Starting in FY 2018, D&D will be funded using indirect funds. Despite budget constraints in past years, excess-facility elimination and disposition remains a Laboratory priority. Table 6-4 provides the projected excess-facility-disposition square footage over the next five years.

**Table 6-1. Summary of projected excess-facility disposition**

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<tr>
<th>Excess Property Type</th>
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<th>2019</th>
<th>2020</th>
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<td>53,275</td>
<td>3</td>
<td>46,608</td>
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**Manage Waste Liabilities**

DOE-NE and DOE-EM have complementary infrastructure to support INL’s waste-management activities. Both organizations have waste-storage pads and waste-disposition infrastructure that directly support their individual missions, and both actively utilize each other’s capabilities when needed to ensure minimal duplication of infrastructure. DOE-NE owns 11 waste-management facilities that directly support the management or handling of newly generated waste from ongoing operations, including R&D programs. DOE-NE uses some of the 25 DOE-EM-owned waste-management facilities where it is not cost-effective to maintain duplicative capabilities or when DOE-NE’s waste stream is small compared to DOE-EM’s waste volumes.

DOE-NE, with NR, is currently constructing a replacement facility for onsite disposal of remote-handled low-level nuclear waste (RH-LLW). DOE-EM will maintain the existing onsite RH-LLW disposal capability until the existing disposal facility is full. Expected to be operational in 2019, the RH-LLW Disposal Facility will be a Hazard Category 2 nuclear facility, consisting of below-grade, precast concrete vaults designed to emplace and dispose of stored and newly generated RH-LLW from ongoing operations, including R&D programs. To address current and future waste-liability issues at INL, additional infrastructure options are being considered and include:

- Enhanced treatment capability for remote-handled bulk-reactives waste generated in future TREAT operations, for future fast-reactor research, and in support of Remote Waste Disposition Project backlog
- Capability for treatment of remote-handled mixed low-level nuclear waste with Resource Conservation and Recovery Act metals (>50R) to support current and future missions
- Waste storage, handling and characterization facilities at MFC to relieve HFEF, the Analytical Laboratory, and various research facilities of waste-storage burden
- Upgrade the Sodium Components Maintenance Shop’s capability to treat and/or prepare difficult contact-handled mixed low-level reactives waste for shipment to off-site treatment facilities.
Optimize Space and Land-use Decisions

Space and land resources are strategically targeted for development to make sure INL can meet growth needs, while maintaining a focus on nuclear energy research first. Decisions are guided by the DOE Asset Management Plan, Laboratory Agenda, and INL business-portfolio planning processes. Hand in hand with attending to the condition of real-property assets is an emphasis on ensuring the most efficient and effective space utilization while providing INL employees with a modern, collaborative, and sustainable work environment that is flexible by design to meet specific program and project needs. A primary tenet is to utilize existing assets to the fullest before considering an asset for excess or before proposing addition of new assets.

To optimize use of space, INL enforces office standards and offers a variety of workspace types and sizes for staff. With the help of PNNL, new space metrics are under development to provide better utilization and return-on-investment data. This, combined with results from walk-downs, has enabled the development of a draft five-year strategic space plan for the REC campus that will focus on consolidating and co-locating support personnel, identifying possible solutions to divest of poorer-condition assets (i.e., the Information Operations and Research Center and the North Holmes Laboratory), and accommodating anticipated growth in other areas. MFC and ATR will be incorporated into the plan next year.

Land-use decisions are governed by a Land Use Committee, comprising senior staff from organizations and contractors supporting missions at INL. The committee is chartered to look at the reasonable arrangement of different INL Site and REC land-use areas and spatial layout to achieve desired objectives. These efforts study proposals, results of suitability evaluations, land-management regulations, and potential program conflicts for purposes of advising and recommending land-use positions. Goals include improving the efficiency and effectiveness of INL land use, maintaining the relative balance of the ecosystem, and achieving sustainable use of resources. The process requires dealing with many correlating factors.

The Idaho National Laboratory Comprehensive Land Use and Environmental Stewardship Report (INL/EXT-15-00726) provides a description of historical land use, current operations, and projected land-use plans. The report is updated when required. It examines multiple land-use options by describing site issues, capabilities, opportunities, and limitations. The land that makes up the INL Site has experienced a long and varied history that ranges from prehistoric times, when it was inhabited by nomadic groups of Native Americans, to its modern use as the location of a world-class nuclear-research center. This represents unique challenges and complexities; major factors governing land-use decisions include the following:

The Comprehensive Environmental Response, Compensation, and Liability Act, commonly known as Superfund, was enacted by Congress on Dec. 11, 1980, and governs environmental remediation, including remediation of federal facilities at the Site.

INL Site was placed on the National Priorities List in November 1989. This required DOE to enter into a Federal Facility Agreement and Consent Order with the EPA and the state of Idaho for effective management of INL Site.

A Settlement Agreement was signed on October 16, 1995, to resolve issues with the state of Idaho related to spent nuclear fuel and waste management. It also recognizes DOE’s commitment under the consent order to complete all major environmental-restoration activities for INL Site.

Operations are governed by hazardous-waste and air-quality permits issued by the state of Idaho.

A Candidate Conservation Agreement was made between DOE and the U.S. Fish and Wildlife Service for rangeland-fire management as a critical priority for protecting, conserving, and restoring the health of the sagebrush-steppe ecosystem and greater sage-grouse habitat.
Historic archaeological sites and artifacts require preservation efforts.

Proximity to nearby cities and towns, a Native American Reservation, and National Wildlife Refuge must be considered.

A good-faith effort is made to enhance the DOE lands through pollinator-friendly best management practice implementation.

Proposals under current or slated for future consideration include the following:

Siting for commercial parties, such as the Carbon Free Power Project small modular reactors, and a possible new fast research reactor

Long-term stewardship of aged federal properties on the REC campus, including the INL Research Center (IF-602/603, 30 years old, 46,512 ft² offices and 112,276 ft² adjacent wet and dry laboratory space), and the Information Operations and Research Center (IF-608, 47 years old, 37,299 ft²)

Expected responsibility for long-term stewardship of the INL Site once the EM cleanup mission is complete

Relocation of fabrication and machining capability from the North Holmes Laboratory

Expansion of the National Security Test Range.
APPENDIX 1

SCIENCE AND ENERGY CORE CAPABILITIES

The Programs reporting to the Under Secretary for Science and Energy have together identified twenty four categories of core capabilities that comprise the scientific and technological foundation of its national laboratories. There are three criteria to define core capabilities. They must:

- Encompass a substantial combination of facilities and/or teams of people and/or equipment;
- Have a unique and/or world-leading component; and
- Be relevant to a discussion of DOE/NNSA/DHS missions.

Below is a table of the core capabilities that have been affirmed by DOE at each of the thirteen Science and Energy national laboratories. The following pages give a detailed definition of what each core capability encompasses.

Figure 1. Distribution of Core Capabilities across the Science and Energy Laboratories

<table>
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<th>Core Capabilities</th>
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<th>BNL</th>
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1. **Accelerator Science and Technology**: The ability to conduct experimental, computational, and theoretical research on the physics of particle beams and to develop technologies to accelerate, characterize, and manipulate particle beams in accelerators and storage rings. The research seeks to achieve fundamental understanding beyond current accelerator and detector science and technologies to develop new concepts and systems for the design of advanced scientific user facilities.

2. **Advanced Computer Science, Visualization, and Data**: The ability to have a widely-recognized role in advances in all applications in computational science and engineering. A core capability in these areas would involve expertise in areas such as programming languages, high-performance computing tools, peta- to exa-scale scientific data management and scientific visualization, distributed computing infrastructure, programming models for novel computer architectures, and automatic tuning for improving code performance, with unique and/or world-leading components in one or more of these areas. The capability requires access to (note: these resources do not need to be co-located) a high end computational facility with the resources to test and develop new tools, libraries, languages, etc. In addition, linkages to application teams in computational science and/or engineering of interest to the Department of Energy and/or other Federal agencies would be beneficial to promptly address needs and requirements of those teams.

3. **Applied Materials Science & Engineering**: The ability to conduct theoretical, experimental, and computational research to understand and characterize materials with focus on the design, synthesis, scale-up, prediction and measurement of structure/property relationships, the role of defects in controlling properties, the performance of materials in hostile environments to include mechanical behavior and long-term environmental stability, and the large-scale production of new materials with specific properties. The strong linkages with molecular science, engineering, and environmental science provides a basis for the development of materials that improve the efficiency, economy, cost-effectiveness, environmental acceptability, and safety in energy generation, conversion, transmission, and end-use technologies and systems. Primary supporting disciplines and field include materials synthesis, characterization, and processing; chemical and electrochemistry, combinatorial chemistry, surface science, catalysis, analytical and molecular science; and computation science.

4. **Applied Mathematics**: The ability to support basic research in the development of the mathematical models, computational algorithms and analytical techniques needed to enable science and engineering-based solutions of national problems in energy, the environment and national security, often through the application of high-performance computing. Laboratory capabilities in this area would involve expertise in such areas as linear algebra and nonlinear solvers, discretization and meshing, multi-scale mathematics, discrete mathematics, optimization, complex systems, emergent phenomena, and applied analysis methods including but not limited to analysis of large-scale data, uncertainty quantification, and error analysis.

5. **Biological and Bioprocess Engineering**: Applies understanding of complex biological systems and phenomena to design, prototype, test and validate processes components, technologies and systems relevant to (1) bioenergy production, (2) environmental contaminants processing, and (3) global carbon cycling and biosequestration. Primary supporting disciplines include chemical engineering, agricultural science, fermentation science, materials science and engineering, and systems science.

6. **Biological Systems Science**: The ability to address critical scientific questions in understanding complex biological systems via the integration of laboratory-specific research facilities, instrumentation and/or leadership-class computational systems, and individuals with expertise in biological systems research and related disciplines to advance DOE missions in energy, climate, and the environment. This unique combination of tools and people is the foundation for research of scale and breadth unmatched by other facilities world-wide, for example, on research that employs systems and synthetic biology and
computational modeling approaches enabled by genome sequencing and functional characterization of microbes, plants, and biological communities relevant to (1) bioenergy production, (2) carbon/nutrient cycling in terrestrial environments and (3) microbial biogeochemical controls on contaminant transport and biosequestration at DOE sites. Primary supporting disciplines include systems biology, plant biology, microbiology, biochemistry, biophysics and computational science.

7. Chemical Engineering: The ability to conduct applied chemical research that spans multiple scales from the molecular to macroscopic and from picoseconds to years. Chemical engineering translates scientific discovery into transformational solutions for advanced energy systems and other U.S. needs related to environment, security, and national competitiveness. The strong linkages between molecular, biological, and materials sciences, engineering science, and separations, catalysis and other chemical conversions provide a basis for the development of chemical processes that improve the efficiency, economy, competitiveness, environmental acceptability, and safety in energy generation, conversion, and utilization. A core capability in chemical engineering would underpin R&D in various areas such as nanomanufacturing, process intensification, biomass utilization, radiochemical processing, dielectric materials, advanced conducting materials, high-efficiency clean combustion, and would generate innovative solutions in alternative energy systems, carbon management, energy-intensive industrial processing, nuclear fuel cycle development, and waste and environmental management.

8. Chemical and Molecular Science: The ability to conduct experimental, theoretical, and computational research to fundamentally understand chemical change and energy flow in molecular systems that provide a basis for the development of new processes for the generation, storage, and use of energy and for mitigation of the environmental impacts of energy use. Areas of research include atomic, molecular and optical sciences; gas-phase chemical physics; condensed phase and interfacial molecular science; solar photochemistry; photosynthetic systems; physical biosciences; catalysis science; separations and analytical science; actinide chemistry; and geosciences.

9. Climate Change Sciences and Atmospheric Science: The ability to apply knowledge of atmospheric, oceanic, terrestrial, ecological, hydrological, and cryospheric processes, that combine with human activities and anthropogenic emissions, in order to understand and predict climate change and different patterns of meteorological conditions, with a particular focus on (1) understanding and describing the causes, impacts, and predictability of climate change via the integration of laboratory-specific research facilities, instrumentation and/or leadership-class computational systems, and individuals with expertise in future climate change research and related disciplines. This unique combination of tools and people is the foundation for research of scale and breadth unmatched by other facilities, world-wide, for example, on (1) atmospheric-process research and modeling, including clouds, aerosols, and the terrestrial carbon cycle; (2) climate change modeling at global to regional scales; (3) research on the effects of climate change on ecosystems; and (4) integrated analyses of climate change, from causes to impacts changes, including impacts on energy production, use, and other human systems, (2) understanding and predicting future extreme weather as the climate evolves, that in turn introduces risk and vulnerability to energy and related infrastructures, (3) understanding the carbon cycle, with focus on the interdependence of a changing climate and terrestrial ecosystems, and (4) predict the influences of terrain and atmospheric processes and systems on the availability, behavior, and quality of energy resource and operations.

10. Computational Science: The ability to connect applied mathematics and computer science with research in scientific disciplines (e.g., biological sciences, chemistry, materials, physics, etc.). A core capability in this area involves expertise in applied mathematics, computer science and in scientific domains with a proven record of effectively and efficiently utilizing high performance computing resources to obtain significant results in areas of science and/or engineering of interest to the Department of Energy and/or other Federal agencies. The individual strengths in applied mathematics, computer science and in
scientific domains in concert with the strength of the synergy between them is the critical element of this core capability.

11. **Condensed Matter Physics and Materials Science**: The ability to conduct experimental, theoretical, and computational research to fundamentally understand condensed matter physics and materials sciences that provide a basis for the development of materials that improve the efficiency, economy, environmental acceptability, and safety in energy generation, conversion, transmission, and utilization. Areas of research include experimental and theoretical condensed matter physics, x-ray and neutron scattering, electron and scanning probe microscopies, ultrafast materials science, physical and mechanical behavior of materials, radiation effects in materials, materials chemistry, and bimolecular materials.

12. **Cyber and Information Sciences**: The disciplines, technologies, and practices designed to protect, analyze, and disseminate information from electronic sources, including computer systems, computer networks, and sensor networks. A core competency in this area would involve recognized expertise in one or more of the following topics: cyber security, information assurance, information analytics, knowledge representation, and information theory, control systems design and engineering, embedded systems, reverse engineering, and advanced hacking techniques. This core competency would be applied to: the protection of information systems and data from theft or attack; the collection, classification, analysis, and sharing of disparate data; and the creation of knowledge from heterogeneous information sources; securing control systems integrated into critical infrastructure; and increasing security, reliability, and resilience of automated processes and systems.

13. **Decision Science and Analysis**: Derives knowledge and insights from measured and modeled data sets to further the understanding of and tradeoffs among resource and technology options, to identify and quantify the risks and impacts of current and emerging technologies on environmental systems, and to assess the impact of market dynamics, human behavior and regulations, policies or institutional practices on the development and uptake of technology. Primary supporting disciplines include engineering, environmental science, applied math, finance, business, social and political science, and market and behavioral economics. This capability provides credible and objective information to support DOE and others to support strategic planning and program direction, policy formulation and implementation, efforts to remove market barriers to deployment and engagement with stakeholders.

14. **Earth Systems Science and Engineering**: The ability to understand environmental and ecological systems, processes, and interrelationships to predict, assess, and mitigate the impacts of past, current, and future energy production, transmission, distribution, and use on subsurface, terrestrial, coastal, and marine environments. Knowledge is used to develop technologies that minimize emissions and/or control technologies that protect these environments.

15. **Environmental Subsurface Science**: The ability to understand and predict the physical, chemical, and biological structure and function of subsurface environments to enable systems-level environmental prediction and decision support related to the sustainable development of subsurface resources, environmentally-responsible use of the subsurface for storage, and effective, mitigation of the impacts of environmental contamination from past nuclear weapons production and provide a scientific basis for the long-term stewardship of nuclear waste disposal via the integration of laboratory-specific research facilities, instrumentation and/or leadership-class computational systems, and multidisciplinary teams of individuals with expertise in environmental subsurface science and related disciplines in microbial ecology and biogeochemistry. This unique combination of tools and expertise is the foundation for research on (1) linking research across scales from the molecular to field scale, (2) integration of advanced computer models into the research and (3) multidisciplinary, iterative experimentation to understand and nutrient cycling and contaminant transport in complex subsurface environments. This
ability can contribute to mitigating the impacts of environmental contamination from past nuclear weapons production and provide a scientific basis for the long-term stewardship of nuclear waste disposal, as well as understanding subsurface environments and their role in the functioning of terrestrial ecosystems.

16. Large-Scale User Facilities/R&D Facilities/Advanced Instrumentation: The ability to conceive, design, construct and operate leading-edge specialty research facilities available to universities, industry, and national laboratories customers to conduct groundbreaking research and development activities and/or ‘at scale’ testing and demonstration of technology. This includes the ability to manage effectively construction of $100 million or greater one-of-a-kind scientific facilities, and to host hundreds to thousands of U.S. and international users in addition to carrying out world-class research at the facility itself. The ability to conceive, design, build, operate and use first-in-class technical instruments intended for a particular research purpose, often requiring the material expertise of multiple scientific disciplines. Instrumentation that can be created by a small number of individuals or that would sit on a laboratory bench-top is not considered part of this core capability.

17. Mechanical Design and Engineering: Applies the principles of physics, mechanics, and materials science to analyze, design, test, validate, and enable operation of advanced engineered systems, machines and tools. Includes equipment used to move or extract energy bearing materials (e.g., oil, gas, coal) or from moving fluids (e.g., water, wind, steam), as well as equipment used to convert energy to useful services (e.g., mobility, home heating and cooling, robotics, imaging devices, etc.) or to manufacture products. Primary supporting disciplines include physics, materials science, aerospace engineering, mechanical engineering, chemical engineering, electrical engineering and computational science.

18. Nuclear Engineering: The ability to use a broad range of facilities, instrumentation, equipment and, often, interdisciplinary teams that apply the knowledge, data, methods, and techniques of nuclear engineering, mechanical engineering, nuclear reactor physics, measurable science and risk assessment to missions of the Departments of Energy and Homeland Security. The elements of this capability are often brought together in unique combinations with those of other disciplines to address high priority needs such as new and improved energy sources and systems; advanced instrumentation for nuclear systems; accelerator science and technology; and development of methods and systems to assure nonproliferation and combat terrorism.

19. Nuclear Physics: The ability to carry out experimental and theoretical research to provide new insights and advance our knowledge on the nature of matter and energy. This includes the design, operation and analysis of experiments to establish the basic properties of hadrons, atomic nuclei, and other particles, and the development of models and theories to understand these properties and behaviors in terms of the fundamental forces of nature.

20. Nuclear and Radio Chemistry: The ability to use a broad range of facilities, instrumentation, equipment and, often, interdisciplinary teams that apply the knowledge, data, methods, and techniques of nuclear chemistry, mechanical engineering, chemical engineering to missions of the Departments of Energy and Homeland Security. The elements of this capability are often brought together in unique combinations with those of other disciplines to address high priority needs such as new and improved nuclear systems; radioisotope production and advanced instrumentation for nuclear medicine; development of methods and systems to assure nonproliferation and combat terrorism; and environmental studies, monitoring, and remediation.

21. Particle Physics: The ability to carry out experimental and theoretical research to provide new insights and advance our knowledge on the nature of matter and energy, and the basic nature of space and time itself. This includes the design, operation and analysis of experiments to discover the elementary
constituents of matter and energy and probe the interactions between them and the development of models and theories to understand their properties and behaviors.

22. **Plasma and Fusion Energy Sciences**: The ability to conduct world-leading plasma research that can range from low-temperature to high temperature/high pressure plasmas. This ability can be in operation of the state-of-the-art experimental fusion facilities to carry out world-leading research on the fundamental physics of plasmas, in theory and computations, which is critical to the full understanding of the plasma phenomena being studied or to enable technologies that allow experiments to reach and in many cases exceed their performance goals.

23. **Power Systems and Electrical Engineering**: Applies understanding of electromagnetic phenomena to design and engineer circuitry, electrical and electronic devices and equipment, sensors, instruments and control systems to address the efficiency and reliability of power transmission and distribution systems, and the interface of the grid with variable generation and modern loads. Primary supporting disciplines include electrical engineering, power systems engineering, computational science, and materials synthesis, characterization and processing.

24. **Systems Engineering and Integration**: The ability to solve problems holistically from the concept and design phase to ultimate deliverable and completion phase, by synthesizing multiple disciplines, and to develop and implement optimal solutions. The ability to develop solutions that address issues of national energy and environmental security. Areas of application of this capability include development of programs in energy supply, storage, transportation, and efficiency; and deployment of novel solutions to materials and sensor problems in fields of interest to the Department of Energy and/or the Department of Homeland Security.
APPENDIX 2
LIST OF DOE/NNSA/DHS MISSIONS

Scientific Discovery and Innovation (SC)

Advanced Scientific Computing Research

1. To develop mathematical descriptions, models, methods, and algorithms to accurately describe and understand the behavior of complex systems involving processes that span vastly different time and/or length scales.

2. To develop the underlying understanding and software to make effective use of computers at extreme scales.

3. To transform extreme scale data from experiments and simulations into scientific insight.

4. To advance key areas of computational science and discovery that further advance the missions of the Office of Science through mutually beneficial partnerships.

5. To deliver the forefront computational and networking capabilities to extend the frontiers of science.

6. To develop networking and collaboration tools and facilities that enable scientists worldwide to work together.

Basic Energy Sciences

7. Discover and design new materials and molecular assemblies with novel structures, functions, and properties, and to create a new paradigm for the deterministic design of materials through achievement of atom-by-atom and molecule-by-molecule control

8. Conceptualize, calculate, and predict processes underlying physical and chemical transformations, tackling challenging real-world systems – for example, materials with many atomic constituents, with complex architectures, or that contain defects; systems that exhibit correlated emergent behavior; systems that are far from equilibrium; and chemistry in complex heterogeneous environments such as those occurring in combustion or the subsurface

9. Probe, understand, and control the interactions of phonons, photons, electrons, and ions with matter to direct and control energy flow in materials and chemical systems

10. Conceive, plan, design, construct, and operate scientific user facilities to probe the most fundamental electronic and atomic properties of materials at extreme limits of time, space, and energy resolution through x-ray, neutron, and electron beam scattering and through coherent x-ray scattering. Properties of anticipated new x-ray sources include the ability to reach to the frontier of ultrafast timescales of electron motion around an atom, the spatial scale of the atomic bond, and the energy scale of the bond that holds electrons in correlated motion with near neighbors
11. Foster integration of the basic research conducted in the program with research in NNSA and the DOE technology programs, the latter particularly in areas addressed by Basic Research Needs workshops supported by BES in the areas of the hydrogen economy, solar energy utilization, superconductivity, solid-state lighting, advanced nuclear energy systems, combustion of 21st century transportation fuels, electrical-energy storage, geosciences as it relates to the storage of energy wastes (the long-term storage of both nuclear waste and carbon dioxide), materials under extreme environments, and catalysis for energy applications.

**Biological and Environmental Research**

12. Obtain new molecular-level insight into the functioning and regulation of plants, microbes, and biological communities to provide the science base for cost-effective production of next generation biofuels as a major secure national energy resource.

13. Understand the relationships between climate change and Earth’s ecosystems, develop and assess options for carbon sequestration, and provide science to underpin a fully predictive understanding of the complex Earth system and the potential impacts of climate change on ecosystems.

14. Understand the molecular behavior of contaminants in subsurface environments, enabling prediction of their fate and transport in support of long term environmental stewardship and development of new, science-based remediation strategies. Understanding the role that biogeochemical processes play in controlling the cycling and mobility of materials in the subsurface and across key surface-subsurface interfaces in the environment enabling the prediction of their fate and transport.

15. Make fundamental discoveries at the interface of biology and physics by developing and using new, enabling technologies and resources for DOE’s needs in climate, bioenergy, and subsurface science.

16. Operate scientific user facilities that provide high-throughput genomic sequencing and analysis; provide experimental and computational resources for the environmental molecular sciences; and resolve critical uncertainties about the role of clouds and aerosols in the prediction of climatic process.

**Fusion Energy Sciences**

17. Advance the fundamental science of magnetically confined plasmas to develop the predictive capability needed for a sustainable fusion energy source.

18. Support the development of the scientific understanding required to design and deploy the materials needed to support a burning plasma environment.

19. Pursue scientific opportunities and grand challenges in high energy density plasma science to explore the feasibility of the inertial confinement approach as a fusion energy source, to better understand our universe, and to enhance national security and economic competitiveness.

20. Increase the fundamental understanding of basic plasma science, including both burning plasma and low temperature plasma science and engineering, to enhance economic competitiveness, and to create opportunities for a broader range of science-based applications.

**High Energy Physics**

21. Understand the properties and interactions of the elementary particles and fundamental forces of nature from studies at the highest energies available with particle accelerators.

22. Understand the fundamental symmetries that govern the interactions of elementary particles from studies of rare or very subtle processes, requiring high intensity particle beams, and/or high precision, ultra-sensitive detectors.

23. Obtain new insight and new information about elementary particles and fundamental forces from observations of naturally occurring processes -- those which do not require particle accelerators.
24. Conceive, plan, design, construct, and operate forefront scientific user facilities to advance the mission of the program and deliver significant results.

25. Steward a national accelerator science program with a strategy that is drawn from an inclusive perspective of the field; involves stakeholders in industry, medicine and other branches of science; aims to maintain core competencies and a trained workforce in this field; and meets the science needs of the SC community.

26. Foster integration of the research with the work of other organizations in DOE, in other agencies and in other nations to optimize the use of the resources available in achieving scientific goals.

**Nuclear Physics**

27. To search for yet undiscovered forms of nuclear matter and to understand the existence and properties of nuclear matter under extreme conditions, including that which existed at the beginning of the universe.

28. Understand how protons and neutrons combine to form atomic nuclei and how these nuclei have emerged during the 13.7 billion years since the origin of the cosmos.

29. Understand the fundamental properties of the neutron and the neutrino, and how these illuminate the matter-antimatter asymmetry of the universe and physics beyond the Standard Model.

30. Conceive, plan, design, construct, and operate forefront national scientific user facilities for scientific and technical advances which advance the understanding of nuclear matter and result in new competencies and innovation. To develop new detector and accelerator technologies that will advance NP mission priorities.

31. Provide stewardship of isotope production and technologies to advance important applications, research and tools for the nation.

32. Foster integration of the research with the work of other organizations in DOE, such as in next generation nuclear reactors and nuclear forensics, and in other agencies and nations to optimize the use of the resources available in achieving scientific goals.

**Workforce Development for Teachers and Scientists**

33. Increase the pipeline of talent pursuing research important to the Office of Science.

34. Leveraging the unique opportunities at DOE national laboratories to provide mentored research experiences to undergraduate students and faculty.

35. Increase participation of under-represented students and faculty in STEM programs.

36. Improve methods of evaluation of effectiveness of programs and impact on STEM workforce.

**Energy Security (ES)**

1. Supply - Solar
2. Supply - Nuclear
3. Supply - Water
4. Supply - Wind
5. Supply - Geothermal
6. Supply - Natural gas
7. Supply - Coal
8. Supply - Bioenergy/Biofuels
9. Supply - Carbon capture and storage
10. Distribution - Electric Grid
11. Distribution - Hydrogen and Gas Infrastructure
12. Distribution - Liquid Fuels
13. Use - Manufacturing Technologies (including efficiency and conservation)
14. Use - Advanced Building Systems (including efficiency and conservation)
15. Use – Transportation Technologies (including efficiency and conservation)
16. Energy Systems Assessment/Optimization

**Office of Fossil Energy (FE)**

1. Develop cost effective carbon dioxide capture technologies applicable to power generation and industrial sources
2. Develop and demonstrate safe, permanent, cost effective carbon dioxide storage and reuse options.
3. Develop advanced fossil based energy conversion technology, such as oxy-combustion, fuel cells, gasification, supercritical carbon dioxide Brayton cycles.
4. Develop crosscutting technologies such as sensors, severe environment material development, and computation modeling tools that support the mission
5. Secure and environmentally sound energy future through responsible production and delivery of our nation’s diverse oil and natural gas resources.

**Environmental Management (EM)**

1. Facility D&D
2. Groundwater and Soil Remediation
3. Waste Processing

**Nuclear Energy (NE)**

1. Improve the reliability and performance, sustain the safety and security, and extend the life of current reactors by developing advanced technological solutions
2. Meet the Administration's energy security and climate change goals by developing technologies to support the deployment of affordable advanced reactors.
3. Optimize energy generation, waste generation, safety, and nonproliferation attributes by developing sustainable nuclear fuel cycles.
4. Enable future nuclear energy options by developing and maintaining an integrated national RD&D framework.
5. Maintain U. S. leadership at the international level by engaging nations that pursue peaceful uses of nuclear energy

**National Security (NNSA)**

1. Stockpile Stewardship and Nuclear Weapons Infrastructure
2. Nonproliferation
3. Nuclear Propulsion

**Homeland Security (DHS)**
1. Border Security
2. Cargo Security
3. Chemical/Biological Defense
4. Cyber Security
5. Transportation Security
6. Counter-IED
7. Incident Management
8. Information Sharing
9. Infrastructure Protection
10. Interoperability
11. Maritime Security
12. Human Factors

**Office of Technology Transitions (TT)**
1. Expand the commercial impact of DOE’s research, development, demonstration and deployment portfolio in the short, medium and long-term in order to advance the economic, energy, and national security interests of the country.
2. Increase the commercial impact of DOE investments through the transition of national laboratory-developed technologies into the private sector.
3. Increase the commercial impact of DOE investments through private sector utilization of national laboratory facilities and expertise.
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