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# ARGONNE NATIONAL LABORATORY

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## Lab-at-a-Glance

**Location:** Lemont, Illinois  
**Type:** Multi-program Laboratory  
**Contractor:** UChicago Argonne, LLC  
**Site Office:** Argonne Site Office  
**Website:** [www.anl.gov](http://www.anl.gov)

- **FY 2018 Lab Operating Costs:** \$782 million
- **FY 2018 DOE/NNSA Costs:** \$672 million
- **FY 2018 SPP (Non-DOE/Non-DHS) Costs:** \$82 million
- **FY 2018 SPP as % Total Lab Operating Costs:** 14%
- **FY 2018 DHS Costs:** \$28 million

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### Physical Assets:

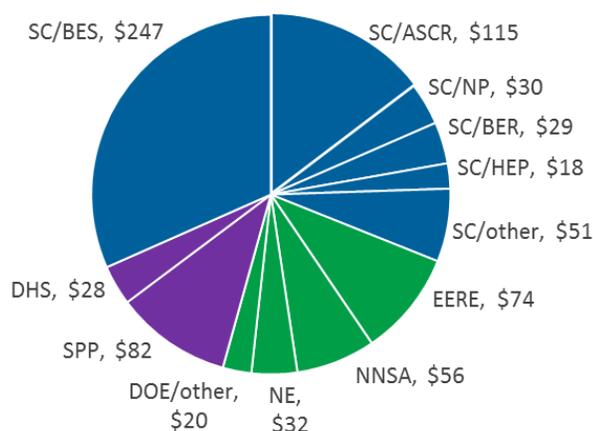
- 1,517 acres and 154 buildings
- 5.0 million GSF in buildings
- Replacement Plant Value: \$3.8B
- 0.02 million GSF in 16 Excess Facilities
- 0.3 million GSF in Leased Facilities

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### Human Capital:

- 3,237 Full Time Equivalent Employees (FTEs)
- 343 Joint Faculty
- 260 Postdoctoral Researchers
- 270 Graduate Student
- 325 Undergraduate Students
- 7,921 Facility Users
- 790 Visiting Scientists

### FY 2018 Costs by Funding Source (\$M)



## Mission and Overview

Argonne National Laboratory accelerates science and technology to drive US prosperity and security. Based in the Chicago suburbs since 1946, Argonne is managed for the US Department of Energy (DOE) by the University of Chicago (UChicago) through UChicago Argonne, LLC.

The Laboratory conducts research that spans the spectrum from basic science to engineering solutions that change the world for the better. Argonne's scientists and engineers are recognized nationally and internationally for leadership in:

- Creating new knowledge through pivotal discoveries in chemistry; materials; nuclear and particle physics; and life, climate, and earth system sciences
- Driving advances in computation and analysis to solve the most challenging problems
- Shaping the nation's future through engineering of advanced technological systems

We build on our discoveries and innovations to improve energy production, storage, and distribution; protect critical infrastructure; and strengthen national security.

The powerful capabilities of our Advanced Photon Source (APS) and Argonne Leadership Computing Facility (ALCF) propel breakthroughs across our broad research portfolio. We are upgrading both of these flagship user facilities, which also serve external researchers: the ALCF will deploy the nation's first exascale computer in 2021 and the APS will be the world's leading hard x-ray microscope by 2025. Three additional major facilities accelerate scientific progress by Argonne and external researchers: the Argonne Tandem Linear Accelerator System, Atmospheric Radiation Measurement Climate Research Facility's Southern Great Plains Site, and Center for Nanoscale Materials. Together, these five facilities serve one of the largest scientific user communities in the DOE complex.

A diverse network of partnerships enriches Argonne's work and enhances the value we deliver to America. Those partnerships include research collaborations with UChicago, other leading universities, and other national laboratories as well as technology transfer collaborations with industry. We support the Chicago region and the nation through community outreach and educational opportunities for the next generation of researchers.

Argonne is committed to extending our proud legacy of unlocking science and technological frontiers to secure America's energy future and deliver economic growth.

## Core Capabilities

Argonne's broad base of expertise in science and engineering, which comprises 18 of the 24 core capabilities defined by DOE for its laboratories, is a powerful asset to meet key national needs for scientific and technological leadership. We use these capabilities to advance the missions of our sponsors as we accelerate science and technology to drive US prosperity and security.

Our multifaceted R&D portfolio enables our scientists and engineers to deliver groundbreaking discovery science and innovative solutions to critical challenges in energy, security, and infrastructure. Our collaborations with UChicago, other universities, other DOE laboratories, and industry enrich our contributions to the nation.

Partnerships with UChicago are integral to our research programs. These partnerships include long-standing collaborations between individual researchers as well as enterprise-level collaborations. Examples of the latter include the Center for Molecular Engineering (CME), an Argonne-based partner to UChicago's Pritzker School of Molecular Engineering, and the Chicago Quantum Exchange (CQE), based in that School. The CQE, an intellectual hub for advancing quantum information science (QIS), is anchored by UChicago, Argonne, Fermilab, and the University of Illinois at Urbana-Champaign. It also includes the University of Wisconsin at Madison, Northwestern University, and six corporate partners.

Another example of an enterprise-level collaboration between Argonne and UChicago is the Joint Task Force Initiative (JTFI), launched in 2018, in which Fermilab also participates. The JTFI includes investments by UChicago in the two laboratories, with the goal of driving development of high-impact research programs that draw on the combined strengths of the three organizations.

Our core capabilities, listed below 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 thousands of researchers from outside Argonne. Those foundational facilities include four on our Illinois site and one in Oklahoma:

- Advanced Photon Source (APS)
- Argonne Leadership Computing Facility (ALCF)
- Argonne Tandem-Linac Accelerator System (ATLAS)
- Atmospheric Radiation Measurement Climate Research Facility's Southern Great Plains (ARM-SGP)

- Center for Nanoscale Materials (CNM)

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Accelerator science and technology	Condensed matter physics and materials science
Advanced computer science, visualization, and data	Cyber and information sciences
Applied materials science and engineering	Decision science and analysis
Applied mathematics	Large-scale user facilities and advanced instrumentation
Biological and bioprocess engineering	Nuclear and radio chemistry
Chemical and molecular science	Nuclear engineering
Chemical engineering	Nuclear physics
Climate change sciences and atmospheric science	Particle physics
Computational science	Systems engineering and integration

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Table: Argonne National Laboratory core capabilities

## Accelerator science and technology

### Capability

Argonne’s accelerator science and technology capabilities center around the APS, ATLAS, and the Argonne Wakefield Accelerator (AWA) and range from electron storage rings and linear accelerators operated as x-ray sources to hadron linear accelerators and advanced accelerator technology. This portfolio of expertise is the foundation for our successful operation of a suite of facilities that support a broad range of scientific research; it also forms the basis for developing enabling technologies for future research and facilities at Argonne and other institutions. Activities among facilities are coordinated and communicated via the Argonne Accelerator Institute.

The nearly 200 Argonne scientists and engineers who work in this field are recognized internationally for their expertise in six areas:

- *Modeling, design, and operation of photon sources, electron accelerators and storage rings, X-ray 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 the APS Upgrade (APS-U) project as well as future X-ray sources at Argonne and elsewhere in the DOE complex
- *Generation, acceleration, and reliable delivery of stable- and rare-isotope ion beams serving nuclear physics research at ATLAS.* We support several DOE and worldwide accelerator initiatives using expertise gained at ATLAS over the past 40 years in linear accelerator design and modeling and in the design and development of state-of-the-art superconducting radio-frequency cavity systems for ion accelerators. We are leveraging our unique expertise and infrastructure for superconducting cavity production, testing, cleaning, and processing to support five major efforts. Those efforts are the APS-U bunch-lengthening system, cryomodule production for the SLAC National Accelerator Laboratory’s Linac Coherent Light Source II, the Proton Improvement Plan II project at Fermilab, the Facility for Rare Isotope Beams at Michigan State University, and R&D for a future electron ion collider
- *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. Using the AWA, we are currently

working to evaluate emittance manipulation techniques in support of future capabilities in photon science. The AWA also is open to the user community for general accelerator R&D in structure and plasma wakefield acceleration, radiation generation, and electron source development.

- *Areas vital to future accelerators and colliders*, including high-power radio frequency sources, generation and preservation of high-brightness beams, photo-injectors, collective beam instabilities, and two-beam acceleration with high transformer ratios. This research is synergistic with our work to improve the performance of light sources and colliders and address national security applications.
- *State-of-the-art accelerator modeling and controls*: our advanced accelerator modeling codes *elegant* and TRACK are used worldwide and we develop EPICS software tools and applications for distributed control systems for accelerators.
- *Support for accelerator outreach, training, and education* via the US Particle Accelerator School based at Fermilab, the summer undergraduate Lee Teng Fellowship in collaboration with Fermilab, and the DOE-funded graduate accelerator education program led by Michigan State University.

### **Mission relevance and funding**

This 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.

## **Advanced computer science, visualization, and data**

### **Capability**

Argonne is a leader in computer science, visualization, and data. We are recognized for our innovation in extreme-scale systems software, scientific software productivity, and high-performance computing tools for data-intensive science. This leadership is critical to achieving DOE's exascale computing objectives.

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

- Foundational computing software and algorithms Foundational computing software 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 the basic and applied sciences
- New concepts and strategies that capitalize on our work in data visualization, analysis, and management for the capture, transport, reduction, transformation, storage, and understanding of data in DOE applications
- 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 high-performance computing
- New fundamental concepts and techniques to support and enhance scientific simulations and data analytics reliability and correctness through advanced resilience, data reduction, and error analysis

Examples of ways in which Argonne's computer science enhances multiple disciplines include the following:

- The SciDAC-4 Rapids Institute for Computer Science and Data is enhancing data analysis capabilities in four strategic research areas:
  - In hard x-ray science: data transfer from APS to ALCF, real-time analysis, and parallel algorithms
  - In materials and chemistry: integrated modeling, analysis, and ultrafast imaging of nanocrystals
  - In physics: high-performance computing analysis of cosmological and accelerator physics models and experiments
  - In applied materials: novel active learning for additive manufacturing
- 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 them in Chicago
- Development of DLHub for materials and chemistry research: This self-service platform for publishing, applying, and creating new machine learning and deep learning models makes it easier for researchers to benefit from advances in those technologies
- Acceleration of data transfer and sharing speeds among DOE laboratories and partners: Advanced data-analysis-informed enhancements to the Globus data management service that increased performance across ESNNet 100-gigabit/second links, in some cases by 50%
- 2018 DOE Early Career Research Program award for research into scalable data-efficient learning for scientific domains
- Two 2018 R&D 100 awards: one for Darshan, a software package for investigating and tuning input-output behavior of high-performance computing applications, and one for Swift/T, a software package for running large workflows on parallel computers

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. Argonne and Fermilab are exploring the future of data storage and networking by leveraging unique Illinois networking infrastructure. 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. We are also involved in managing and executing DOE's research plan for exascale computing, and we maintain partnerships with researchers in Japan and Europe.

### **Mission relevance and funding**

This 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/SC-BER and -BES; NIH; NIST; DOD, and NSF. Much of this additional funding supports co-design activities, basic and applied research, and interdisciplinary research partnerships with scientists in various application areas.

## **Applied materials science and engineering**

### **Capability**

Argonne applies internationally recognized expertise in materials development, synthesis, processing, and scale-up to drive advances in clean energy technologies. Applied and basic science teams from across the Laboratory do this work using a unique suite of resources. Those resources include materials characterization at the APS and CNM; computational science using the ALCF; one-of-a-kind facilities for materials synthesis and for fabrication and testing of components and devices; CME expertise; and process R&D and scale up of materials in our DOE/EERE-funded Materials Engineering Research Facility (MERF).

The capabilities in the MERF enable scientists and engineers to bridge the gap between bench-scale science and industrial implementation. Researchers develop scalable processes and advanced manufacturing techniques to produce innovative materials in sufficient quantities to enable industrial testing and accurate cost modeling.

Argonne is a leader in creating innovative materials and applying those materials to real-world challenges. 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 high-performance applications, including fuel cell catalysts, solid-state lighting, 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 uses such as hydrogen production, biofuels processing, lithium metal manufacture, and water treatment and reuse. An expanding focus is the recovery and reconstruction/upcycling of specialized materials, with the establishment of the DOE/EERE-funded ReCell Center focused on recycling of lithium-ion batteries.

Our applied materials science and engineering has produced more-efficient batteries, new solar panel designs, high-performance sponges for oil adsorption, 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, advanced energy storage devices, and higher-performance superconducting materials for use in detectors, accelerators, and energy transmission.

We are expanding the MERF to provide additional laboratory and collaborative space to enable additional materials manufacturing, synthesis, and processing capabilities for varied application domains.

Argonne's nuclear materials work focuses on verifying the safety of current light-water reactors and developing new materials to improve the economics and enhance the safety of advanced reactors. This research builds on our capability to design and develop materials for extreme conditions and our nuclear engineering capability.

The Argonne Collaborative Center for Energy Storage Science (ACCESS) is facilitating maturation of novel battery materials and their deployment to industry. We also partner with industry through innovative manufacturing institutes, including PowerAmerica, Digital Manufacturing Design and Innovation Institute, and Reducing Embodied-energy and Decreasing Emissions (REMADE).

### **Mission relevance and funding**

This 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. It builds on discoveries in our core capability in condensed matter physics and materials science, with an ultimate goal of moving those discoveries to market. It is aligned with the goals of the DOE Energy Materials Network (EMN) and supports many of the consortia, including the Chemical Catalysis for Bioenergy (ChemCatBio) and Lightweight Materials (LightMat) consortia.

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.

## **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) and provide best-in-class expertise in

automatic and algorithmic differentiation (AD). We also are a recognized leader in mathematical optimization algorithms, modeling, software, and theory. Our strategy for the future emphasizes:

- Creating time- and energy-efficient PDE and optimization solvers for the exascale era and beyond
- Extending and combining AD, data assimilation, optimization, and PDE capabilities to support efficient solution of design, decision, and control problems while accounting for error estimates and uncertainty
- Applying expertise in optimization, statistics, and AD as building blocks for machine learning for scientific applications
- Expanding our capabilities in machine learning, statistics, quantum algorithms, and other strategic areas
- Combining approaches – machine learning, statistics, and optimization – to solve inverse and analysis problems associated with simulation, observation, and experimental data

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

- New scalable computational frameworks for modeling and solving large-scale-optimization-under-uncertainty problems by using high-performance computing for the planning, design, and control of networked systems such as electrical, gas, transportation, and water networks
- New multimodal machine learning, statistical modeling, and algorithmic approaches to analyzing experimental, observational, and simulation data, including APS data and environmental observations
- Automated machine learning, multi-objective optimization, and differentiation algorithms deployed for applications such as urban data analytics, supercomputing performance, and oceanographic modeling and also applied to post-Moore architectural concepts

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 ADIC, OpenAD/F, Rapsodia, and SWIG-PyADOLC AD tools for C, Fortran, Python, and R
- DSP and MINOTAUR, which solve 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 ecosystem, designed to run on the most powerful supercomputers in the world, 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 earth’s geological evolution, and how to cool nuclear reactors efficiently. These capabilities have been recognized by multiple R&D 100 Awards and the naming of staff members as Fellows of the Society for Industrial and Applied Mathematics.

### **Mission relevance and funding**

This capability supports the DOE/SC-ASCR mission to develop and deploy high-performance and leadership computing resources for scientific discovery. Other current sponsors include DOE/ECP; DOE/EERE; DOE/NE; DOE/OE; DOE/SC-BER, -FES, -HEP, and -NP; DARPA; DHS; and NSF: much of this funding entails interdisciplinary research partnerships leveraging applied mathematics expertise.

## Biological and bioprocess engineering

### Capability

Argonne's bioprocess research determines the fundamental engineering mechanisms for biological energy capture and conversion, from the molecular to the unit-operation scale, and uses the results to pioneer first-principles bioengineering approaches. Our new approaches to biological and bioprocess engineering combine synthetic biology and synthetic chemistry to create biomaterials with tuned functionalities.

This capability draws on the CNM, the APS, and Argonne's computational expertise and resources. CNM's tools for imaging and manipulating biomolecules, cells, and processes over multiple scales are used extensively for bioprocessing. We use multiple APS beamlines – including one dedicated to the DOE/SC-BER-funded Structural Biology Center – to determine the crystallographic structure of biological macromolecules and to characterize catalysts in thermochemical conversion processes: associated capabilities include bionanoprobe and micro-diffraction tools. Our Advanced Protein Characterization Facility can produce and characterize tens of thousands of unique proteins each year, including their biophysical and biochemical properties. Our computational expertise and resources have enabled us to be leaders in developing bioinformatic tools for the larger research community.

Current research directions and investments focus on:

- Synthetic biology for biosystems design. We annotate and model microbial and microbiome systems (KBase) to enable discovery of enzyme function, predictive design of strains and communities, and ecological understanding. We integrate this capability with our experimental expertise in protein characterization, structure-based design of proteins, engineering of microbial genomes, and use of biohybrid materials to visualize biological functions in cells and the environment. We are advancing this capability through internal investments, university collaborations, and strategic partnership projects.
- Bioprocesses and biomanufacturing. Our work to improve bioprocesses emphasizes directed molecular evolution for natural and artificial photosynthetic systems, catalyst separation and reuse, bioreactor design and operation from bench to pilot scale, and extraction and separation of biofuel candidates from bioreactors without disruption of bioprocesses. Sustainable plastic design combines efforts across Argonne in data science, environmental science, biology, and soft-matter chemistry. As the lead lab for the DOE/EERE-BETO Bioprocessing Separations Consortium, we have applied ion-adsorbent wafers to directly capture organic salts produced during fermentation and developed and applied nanomaterials that can be used in situ in fermentations to selectively bind toxins or inhibitors and be reused more than 100 times.

Through recent advances in biological and bioprocess engineering, we have demonstrated the ability to predictively engineer microbes from the environment, microbes for biotechnology, energy-converting proteins with radically altered function, and enzymes to transform biomass. This creates a synthetic biology capability to develop designer microbes and communities for fundamental understanding of biological functions, biomanufacturing, and energy-water research, and for linking with biohybrid research by our chemists and material scientists. We couple computational and experimental approaches to facilitate analysis, predictive modeling, and design of microorganisms and environmental microbiomes across scales.

Through the DOE-SC/BER KBase project, we integrate modeling and computational analysis – including metabolic modeling, cheminformatics, omics, and meta-omics – to support bioengineering efforts for microbes, plants, and microbial communities. We also contribute to the development of biomanufacturing technologies as part of the DOE/EERE-BETO Agile Biofoundry project, and are a member of the Feedstock Conversion Interface Consortium initiated by that office. In addition, we are a

leader in lifecycle and techno-economic analyses of bioenergy-related processes and analyses of the impacts of bioenergy system deployment on soil carbon, water footprint, water quality, and landscape design.

### **Mission relevance and funding**

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

## **Chemical and molecular science**

### **Capability**

Chemical and molecular science is central to many of Argonne's research programs. World-leading strengths include chemical characterization of matter, computational and theoretical chemistry, electrochemistry, functional chemistry, interfacial chemistry, mechanistic chemistry, molecular control of chemical transport and chemical reactivity, molecular design and synthesis, and light-matter interactions. Our work explores trends in chemistries across the entire periodic table, and includes expertise in gas phase, liquid phase, and solid-state chemistries. In support of the DOE/SC mission, we have used these strengths to deliver scientific advances relevant to DOE mission needs in catalysis, combustion, electricity production from chemical energy, energy storage, geochemistry, heavy element separations, and solar and photosynthetic processes.

We have unique competencies in ultrafast characterization of reactions, thermochemical analysis, organometallic chemistry combined with heterogeneous catalysis, synthesis of unique physical and chemical environments, characterization of interfaces and interphases, metal ion separations, nuclear coordinate and electronic structure modeling, and cascading gas phase reactions.

The computational resources and characterization tools available through ALCF, APS, and CNM are integral to this capability. Other facilities central to our work include our unique High-Throughput Research Laboratory, atomic layer deposition laboratories, existing and under-construction radiological facilities, and Advanced Electron Paramagnetic Resonance Facility.

The advancement of this capability is enhanced by our engagement with UChicago, particularly through the CME, and with Northwestern University through the Northwestern University – Argonne National Laboratory Institute for Science and Engineering. With both institutions, we recently stood up the Energy Frontier Research Center on Advanced Materials for Energy-Water Systems (AMEWS), which is focused on the science of water/solid interfaces, with an emphasis on molecular separations.

In addition, our core capability in condensed matter physics and materials science complements these strengths through materials design and synthesis and functional material development. We advance our DOE/SC-BES discoveries in chemical and molecular science through collaborations with industry and in conjunction with expertise embodied in our core capabilities in chemical engineering and applied materials science.

Argonne's strategy advances an integrated, systems approach to the chemical and molecular sciences in concert with our chemical engineering and applied materials science and engineering core capabilities. We seek to unify the understanding of the periodic table, taking advantage of our expertise in the chemistry of the light elements, through the transition metals and on to the heavy elements. We seek to understand transient processes within molecules through our ultrafast chemistry and ion and electron transport expertise. Additionally, competing reactions are at the core of our strategy, which seeks to understand the interactions of these competing processes, including the role of rare events and

spectator species. Efforts in understanding dynamics, structure, and transport of complex environments will impact areas such as separations, catalysis, geochemistry, and photochemical processes. Finally, understanding interfaces in dimensions of x, y, z, and time is vital to our work within this core capability.

Looking forward, we are expanding our capabilities in polymer science and advancing investigations on how to predict and control the flow of electrons, ions, and molecules at interfaces relevant to geochemistry, separations, catalysis, electrocatalytic and electrochemical processes, and light-induced processes relevant to solar energy conversion. To address the challenges and opportunities of predictive chemistries, we will further integrate Argonne's expertise in computational, theoretical, and data sciences into experimental chemistry research, based on output from our JTFI work in artificial intelligence for science. Precision synthesis for controlled chemical conversions will continue to be at the fore in addition to the necessary characterization of atoms and molecules spanning length scales from atomic to microns and time scales from ultrafast to seconds under in situ and operando conditions.

During FY20, our DOE/SC-BES heavy elements chemistry and separations science programs will move to the Materials Design Laboratory, which will advance our systems approach by fostering new interdisciplinary science within a state-of-the-art research complex.

### **Mission relevance and funding**

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

## **Chemical engineering**

### **Capability**

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, biomass conversion, chemical and light energy conversion, and water cleanup. This capability integrates chemical engineering expertise with our core capabilities in chemical and molecular science, condensed matter physics and materials science, and biological and bioprocess engineering.

Our success in applying our foundational knowledge in electro-, photo- and thermo- chemistry and catalysis, and in interfacial sciences, has led to global recognition for our lithium-ion (Li-ion) battery, solar conversion, combustion chemistry, and fuel cell research. We are now advancing the next generation of Li-ion batteries, looking beyond Li-ion batteries, developing solid-state batteries and solutions for stationary storage, and advancing methods to recycle Li-ion batteries through our new ReCell Center. Our multidisciplinary efforts are 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. Our high-temperature gas phase chemistry and chemical and material scale-up expertise are leading to new engine designs and pathways for translating DOE/SC discoveries and DOE/EERE-VTO foundational research to meet industry and consumer needs.

In addition, we are accelerating the development of catalysts that do not use platinum-group metals for fuel cells, through the use of high-throughput materials synthesis, characterization, and performance evaluation of equipment and methodologies. This activity is a cornerstone of DOE's ElectroCat research consortium, which we co-lead with Los Alamos National Laboratory. Other efforts are intended to reduce the costs to produce renewable liquid transportation fuels through advances in catalysis and improved approaches to radioisotope processing.

Argonne operates a unique suite of facilities for energy storage and conversion R&D, a suite that is integrated with our process and systems modeling capabilities. Our modeling capabilities include

process unit modeling, performance vs cost modeling, and techno-economic and life cycle analysis.

Facilities include:

- Cell Analysis, Modeling and Prototyping (CAMP) facility. Cells manufactured in this facility enable realistic, consistent, and timely evaluation of candidate battery-cell chemistries in a close-to-realistic industrial format.
- Electrochemical Analysis and Diagnostics Laboratory (EADL). This laboratory provides battery developers with performance evaluation of cells, modules, and battery packs, allowing diagnostic analysis of battery components after use to identify mechanisms that limit battery life.
- Post-Test Facility. This facility is designed to understand failure modes in batteries with air-sensitive materials, such as those from lithium-based or sodium-based battery technologies.
- High-Throughput Research (HTR) Laboratory. This laboratory provides robotic tools and reactor systems for rapid, automated, and parallel approaches to chemical synthesis and materials development, thereby accelerating discovery and optimization of materials for catalysis, energy storage, fuel cells, solar energy, and nanoscale chemistry.
- Materials Engineering Research Facility (MERF). This facility allows researchers to explore the scale up of materials and chemical processes as we work with industry to move national laboratory discoveries and industry innovations to the marketplace. It is described in more detail under our applied materials science and engineering capability.
- Low Energy Accelerator Facility (LEAF). This facility is used for radioisotope processing.

To meet increased needs, we recently updated LEAF and completed a three-fold expansion of CAMP; we currently are expanding MERF. DOE/EERE provides the majority of funding for CAMP, EADL, MERF, Post-Test Facility, and the HTR Laboratory. DOE/NE supports LEAF.

### **Mission relevance and funding**

This capability supports the missions of DOE and other agencies to advance energy storage and fuel cell science and engineering. Current sponsors include DOE/EERE, DOE/NE, DOD, and industry.

## **Climate change sciences and atmospheric science**

### **Capability**

Through research in climate change and atmospheric sciences, Argonne improves understanding of the earth's atmospheric and environmental systems and advances efforts to address climate-related energy, water, and security challenges. The Laboratory makes leading contributions in three areas: atmospheric measurement and analysis, earth science simulations, and soil and biogeochemical science. We are investing in integrating these three areas to develop a predictive understanding of the role of heterogeneity in mediating water, energy, and carbon exchanges in earth systems. This investment leverages a number of Argonne strengths described below.

Argonne's strengths in atmospheric science are grounded in our ability to make sophisticated atmospheric measurements at an unprecedented scale and under challenging circumstances. Today we oversee operational activities across all the ARM sites supported by DOE/SC-BER. In addition, we operate the ARM Southern Great Plains site, which is the world's largest and most extensive research facility for in situ and remote sensing of cloud, aerosol, and atmospheric processes. We also provide the global scientific community with unique expertise and software for atmospheric instrument operation and measurements. Our Py-ART software for radar data is recognized internationally.

We apply our aerosol/cloud science and instrument expertise, along with ARM data, to better understand terrestrial-atmospheric coupling and the role of cloud processes in the hydrologic cycle and

to define the impact of surface- and boundary-layer coupling on low-level clouds. We have made fundamental contributions to the physics of low-level clouds using ARM data and developed novel methods for retrieving atmospheric thermodynamic and cloud properties from data collected by suites of remote sensing instruments.

Argonne's efforts to advance earth science simulation emphasize the application of high-performance computing to develop robust predictive capabilities. We support the computational objectives of DOE's flagship Energy Exascale Earth System Model (E3SM) in addition to the data and analytical needs of other DOE R&D areas related to climate and atmospheric science.

We are developing models that we use in combination with field observations to understand the influence of aerosols and aerosol life cycle on low-level clouds and the earth's radiation budget. For example, we have used this approach to gain valuable insights into the life cycle of aerosols from biomass combustion in Africa, and we continue to incorporate aerosol and dust science into E3SM.

Argonne is an international leader in downscaling earth system modeling results to project possible future local climate conditions. We recently used our 12-km-resolution climate projections for North America to support quantitative analysis of risks to industrial infrastructure from future extreme weather. By combining our projections with regional atmospheric and hydrological models, we estimated the future probability of high winds, heavy precipitation, flooding, and coastal storm surge in the Southeast.

We have collaborated with DOE/EERE-WETO and NOAA to improve the accuracy of numerical weather prediction models over complex terrain, in support of wind-energy production. In this project, Argonne scientists analyzed wintertime cold pool events and boundary layer wind jets and provided three heavily instrumented wind sites and two physics sites that gathered latent and sensible heat flux data.

Using the APS, Argonne pioneered the application of synchrotron technology to perform chemical and physical analyses of atmospheric dust, aerosols, and soils. The APS Upgrade will vastly expand the capabilities of this technology for environmental science.

More broadly, our soil and biogeochemical scientists are developing a deep predictive understanding of soil responses to environmental change and perturbation, from the molecular to the regional scale. We apply microbial ecology to advance knowledge of soil processes, develop novel technologies to characterize soil properties, and use geospatial analytics to extend field measurements.

We have produced spatially explicit estimates of carbon stocks of permafrost-affected soils in the far northern hemisphere, using our pioneering rapid mid-infrared spectroscopy technique to assess the degradation state of organic matter in those soils. This information is vital to predicting future carbon emissions from soils in this vulnerable region. We are also developing novel sensor technology to monitor soil moisture, a critical variable in both soil and atmospheric processes.

### **Mission relevance and funding**

This core capability supports the missions of DOE/SC-BER and other federal entities with climate and atmospheric science initiatives. Additional sponsors include DOE/EERE-WETO, NSF, DOD, NASA, and NSF.

## **Computational science**

### **Capability**

Computational science, a cornerstone of Argonne's R&D enterprise, advances the solution of critical problems in many scientific disciplines. Our Laboratory-wide computational activities involve more than

350 scientists and engineers working in interdisciplinary project teams that include applied mathematicians and computer scientists. Argonne's computational science effort is strongly supported by the capabilities of the ALCF, Joint Laboratory for System Evaluation, and Laboratory Computing Resource Center.

We will continue to enhance and promote our computational science capabilities, in the following ways:

- Leverage our computational science division and data science and learning division to build strong collaborative projects with scientists and engineers across Argonne in modeling, simulation, and machine learning. We are facilitating crosscutting Laboratory-wide engagement in computing and fostering multidisciplinary teams for conducting leading-edge computational science.
- Through our computing divisions, provide computational scientists and engineers with ready access to broad and deep expertise in traditional and emerging scientific computing methods and tools. These methods include modeling and simulation, data science, machine and deep learning, software development and optimization, and next-generation technologies such as quantum and neuromorphic computing.
- Use a matrix model to integrate domain expertise with methodological expertise in computational science, data science, and machine learning.
- Take advantage of the co-location of hardware and staff expertise to strengthen proposals of both internal and external computational science groups as they apply for DOE's Innovative and Novel Computational Impact on Theory and Experiment and ASCR Leadership Computing Challenge awards.

Some examples of the impact and leadership of Argonne's computational science capability follow:

- We performed some of the world's largest high-resolution cosmological simulations with Argonne's HACC code, modeling the universe over billions of years. HACC plays an important role in benchmarks for future DOE computing systems and is a significant part of two major efforts within DOE's Exascale Computing Project (ECP).
- We developed and implemented algorithms and toolkits for analysis of large datasets from Argonne's APS, the Large Hadron Collider in Switzerland, and the Large Synoptic Survey Telescope.
- Our peers have recognized the computational science enabled by our PETSc library with multiple Gordon Bell prizes and the joint prize in Computational Science and Engineering awarded by the Society for Industrial and Applied Mathematics and the Association for Computing Machinery.
- Our NekCEM/NEK5000 code has been used in applications spanning fluid flow, thermal convection, combustion and magnetohydrodynamics. It won an R&D 100 award in 2016 and is used in two application projects within the ECP.
- Argonne staff engage in development of community codes such as NAMD and QMCPACK.
- We participate in 10 SciDAC application partnerships spanning environmental science, fusion, high-energy physics, nuclear physics, and nuclear engineering.
- We developed and contributed to a spectrum of applications: these include elegant (accelerator simulation), TomoPy (x-ray tomographic analysis), and Green's Function Monte Carlo (properties of nuclei). The latter revealed new details of the carbon-12 nucleus structure and is enabling research that will improve understanding of subatomic particles.

### **Mission relevance and funding**

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

# Condensed matter physics and materials science

## Capability

Argonne's internationally recognized condensed matter physics and materials science research predicts, designs, and creates new materials and advances understanding of their behavior. Our leadership in this field relies on the breadth and depth of our expertise in materials chemistry and physics, scattering and imaging, theoretical and computational science, and the integration of APS, CNM, and ALCF capabilities into our work.

Our strategy emphasizes the role of defects and interfaces across three areas: quantum and spin coherent matter, soft matter and hybrid materials, and electrochemical phenomena. We give crosscutting emphases to precision synthesis, in situ and operando studies coupled to modeling and simulation, and nascent AI and data science approaches. We study magnetic, superconducting, and catalytic materials; quantum metamaterials; ferroelectrics; correlated oxides; polymers; topological materials; and electrochemical oxides. The CME is an important element of our strategy; its staff members bring expertise in soft matter and in semiconductor- and superconductor-based QIS platforms.

Our capabilities and tools uniquely position us to deliver scientific breakthroughs. Key assets include materials discovery using high-pressure floating-zone crystal growth and thin-film growth of topological matter and refractory transition metal elements as well as oxychalcogenides, diamond, and aluminum nitride as platforms for discovery in quantum information science. We are innovating in situ characterization approaches, including coherent diffraction, three-dimensional pair-distribution analysis of diffuse x-ray and neutron scattering, terahertz dynamics, and Lorentz microscopy for imaging vector magnetization.

Argonne leads the Midwest Integrated Center for Computational Materials, which is a collaboration with UChicago and four additional universities, and plays a key role in the Center for Predictive Simulation of Functional Materials at Oak Ridge National Laboratory. We also are a leader in simulating vortex dynamics of superconductors, of importance to multiple programs supported by DOE/SC.

Our core materials science reinforces the work of the Argonne-led Joint Center for Energy Storage Research, through our Electrochemical Design Laboratory, and plays a principal role in materials-focused Energy Research Frontier Centers. Those centers include two led by Argonne [Advanced Materials for Energy Water Systems (AMEWS) Center and the Center for Electrochemical Energy Science] and four led by other institutions. UChicago and Northwestern University are partners in the AMEWS Center. We will leverage the ultrafast electron microscope at CNM to explore phenomena such as transient behavior in ferroic nanostructures, structural phase transitions, and phonon interactions.

Our work has had recent impact at frontier areas of science including (1) topological superconductivity in strontium-doped bismuth selenide, (2) critical slowing-of charge order explained through a combination of ultrafast optical and x-ray experiments and dynamical mean field theory, and (3) simultaneous measurement of strain and stacking faults in gallium nitride nanowires using coherent x-ray ptychography. Additional recent impact areas include (1) phonons as a prime candidate mechanism for superconductivity in twisted bilayer graphene, (2) nanomagnetic arrays to encode quantum information into electron beams, (3) novel core-shell iridium oxide structures to understand oxygen reduction reactions, and (4) neutron diffuse scattering as a means to isolate competing interactions in relaxor ferroelectrics.

Looking forward, we will address research and technique-development in coherent x-ray scattering that will help to shape the scientific mission of the upgraded APS, for instance through expanded in situ and operando studies of ionic motion in solids and liquids, accelerated by combining coherent x-ray probes with machine learning.

We will propose new fundamental research to advance materials for the QIS, AI, and data science revolutions. In QIS, we will explore quantum magnonics and structured electron beams and develop new qubit platforms via atomic layer deposition and molecular beam epitaxy approaches to defect creation and control. We also will propose first-principles, simulation-based approaches for predicting synthetic pathways for inorganic solid-state materials. Preparing for Argonne's Aurora exascale computer, we will propose data science approaches built on collaborations among condensed matter physicists, materials scientists, and experts in AI and data science.

During FY20, we will occupy the Materials Design Laboratory, which will provide state-of-the-art infrastructure for quantum, magnetic, superconducting and scattering science programs. Looking ahead, we will develop scientific programs and expertise to shape the planned Sensing and Imaging at Argonne building.

### **Mission relevance and funding**

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

## **Cyber and information sciences**

### **Capability**

Through our cyber and information sciences programs, we protect, analyze, and disseminate information from computer systems and other electronic sources to defend our nation from cyber attacks. This work supports the overall cybersecurity of national infrastructure, including the electric grid, water systems, transportation assets, and supply chains.

We take a collaborative cross-disciplinary approach to address emerging problems in this arena and deliver results of global impact. Internally, our cyber and information sciences activities leverage Argonne's advanced computing and engineering capabilities, including the APS, ALCF, and Laboratory Computing Resource Center. Our external partners include researchers from universities, other national laboratories, and the private sector.

We help protect the nation as a trusted partner to 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. Through our cyber and information sciences strategy, we:

- Conduct proactive cybersecurity research in critical infrastructure risk and resilience, moving target defense, autonomous vehicle security, machine learning for intrusion detection, and other technologies to improve national security
- Share 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, which Argonne runs as DOE's primary system for sharing cyber threat information relative to the Cybersecurity Information Sharing Act of 2015
- Develop capabilities to leverage machine-to-machine information sharing to help cyber defenders hunt for active threats in their networks, collaborate on analysis, and orchestrate their defenses
- Design tools for evaluating the resiliency, dependencies, and defenses of computer systems that operate critical infrastructure, as well as the consequences of attacks on those systems
- Inform government and private-sector entities of potential cyber vulnerabilities through the DHS Regional Resiliency Assessment Program

- Apply cutting-edge research and development to design systems supporting power grid operations that are resilient to the cybersecurity threats of the future, in support of the DOE/CESER Cybersecurity for Energy Delivery Systems program
- Conduct short- and long-term assessments of cyber threats, vulnerabilities, consequences, and dependencies, including trend analyses
- Partner with DOE/CESER to develop and host its annual collegiate CyberForce Competition™, which uses scenarios focused on energy-critical infrastructure to develop the nation's next generation of cyber workforce by increasing students' understanding of cyber-physical threats, vulnerabilities, and consequences
- License Argonne's patented MORE Moving Target Defense technology, recipient of an R&D 100 Award, which enhances cybersecurity through a rotation of multiple operating systems that can be deployed in a production information technology environment
- Deploy advanced algorithms and tools that monitor the physics of the power grid to detect and mitigate attacks on cyber-physical systems

Facilities that support this capability include enterprise data centers that host a multi-agency secure private cloud and state-of-the-art facilities for analyzing vehicle cybersecurity. We currently are investing resources to integrate high-performance computing and dependency modeling as it applies to the cybersecurity mission space.

### **Mission relevance and funding**

This capability supports the missions of DOE, DHS, DOD, and industry. Current DOE sponsors include DOE/CESER, DOE/EERE, DOE/EPSCA, DOE/IN, DOE/NE, DOE/NNSA, and DOE/OCIO. Current DHS sponsors include the Federal Emergency Management Agency, Office of Intelligence and Analysis, and Cybersecurity and Infrastructure Security Agency.

## **Decision science and analysis**

### **Capability**

Argonne is recognized for addressing pressing national challenges in decision science and analysis through development and application of novel modeling approaches. These approaches include agent-based modeling, complex adaptive system modeling, system dynamics, and complex network analysis. We have attained international leadership in the development of high-performance computing software tools (Repast, EMEWS, and PLASMO) and their use in extreme-scale agent-based modeling applications. This capability, linked with our cyber, information science, and systems engineering capabilities, positions us to deliver effective solutions to complex problems that require multidisciplinary solutions.

We approach problems as dynamic and interrelated systems in order to address uncertainty, rapidly changing environments, and imperfect/incomplete data. Combining these models with traditional deterministic methods better informs key decision makers.

Facilities that support this work include an immersive data visualization STUDIO for Augmented Collaboration (STAC) and the ALCF. We have applied leadership computing capabilities to the analysis of social and behavioral systems, including predictive modeling of the spread of infectious disease and information in urban areas and the effectiveness of interventions to mitigate disease spread. Looking to the future, we expect to make increasing use of advanced computing approaches and architectures, including exascale systems, machine learning, and artificial intelligence.

Staff members across multiple Argonne divisions are dedicated to a decision science and analysis strategy in which we:

- Analyze infrastructure assets and systems, with particular emphasis on lifeline sectors and the electric grid, to inform government and private-sector decisions regarding risk mitigation, resilience enhancement, restoration, and recovery in an all-hazards environment. Our infrastructure work also draws on our capabilities in systems engineering and integration. For example, we use predicted hurricane paths in the East Coast and Gulf regions to forecast likely power outages, to facilitate restoration of service
- Extend decision science capabilities beyond our traditional energy infrastructure assessments to address emerging problems in energy-water interdependence and urban sciences
- Develop and deploy models and associated web applications to analyze supply chains, to inform state-wide decision-making by emergency managers in response to expected and unexpected impacts to various systems
- Develop models and conduct analyses of global supply chains to inform decisions affecting the national stockpile of critical materials that support national security and advanced energy technology
- Assess the complex interactions (cascading and escalating) of infrastructure dependencies in local, regional, national, and international systems to inform resilience-enhancement decisions
- Analyze the social dynamics of energy and national security issues to inform decisions pre-, trans-, and post-event for a variety of scenarios
- Apply our expanded Greenhouse gases, Regulated Emissions, and Energy use in Transportation (GREET) life-cycle-analysis model to inform decisions about new technologies and concepts within initiatives such as the DOE/EERE-FCO H2@Scale program
- Use agent-based modeling to model the propagation outcomes of gene editing and gene drive technology through populations over generations

In addition, we are addressing how best to meet future DOE needs for earth system prediction. A scientific challenge is to capture the reverse feedback from human behavior on the environment. Supporting research focuses on model coupling, ensemble modeling, and uncertainty propagation, with the goal of providing model-generated information to decision makers, and on understanding the social dynamics of how information, and misinformation, spreads through social networks. We are collaborating with UChicago researchers in this area.

### **Mission relevance and funding**

This capability supports the missions of DOE, DHS, DOD, and industry. Current DOE sponsors include DOE/CESER, DOE/EERE, DOE/IN, DOE/NE, DOE/NNSA, DOE/OCIO, DOE/OE, and DOE/OP. Current DHS sponsors include the Federal Emergency Management Agency, Cybersecurity and Infrastructure Security Agency, and Office of Intelligence and Analysis.

## **Large-scale user facilities/advanced instrumentation**

### **Capability**

#### *Advanced Photon Source (APS)*

Funded primarily by DOE/SC-BES, the APS is an internationally leading source of high-energy x-rays for scattering, spectroscopy, and imaging studies. Grounded in Argonne's unique blend of expertise in high-energy x-ray science, instrumentation, optics, and accelerator physics, the APS provides unmatched capabilities for studies over a wide range of length and time scales. Capabilities include in situ and operando sample environments; macromolecular crystallography; high-pressure environments and shock physics; x-ray interrogation of electron and lattice excitations; and real-time studies of evolving systems. We have initiated the APS Upgrade project, to create the world's brightest hard x-ray storage-ring light source.

### *Argonne Leadership Computing Facility (ALCF)*

Funded by DOE/SC-ASCR, the ALCF operates two open-science supercomputers, an IBM Blue Gene/Q system (ALCF-2, named Mira) and an Intel/Cray XC40 system (ALCF-Lithium, named Theta), that rank among the 25 fastest machines in the world. The ALCF provides petascale-computing capabilities and support services that enable the computational science and engineering community to run the largest and most complex calculations. ALCF also hosts the Joint Laboratory for System Evaluation, which gives our staff and collaborators access to the latest production and prototype computing resources, and operates a Cray Xeon cluster (named Cooley) used for data analysis. In 2021, the ALCF will deploy DOE's first exascale system, an Intel/Cray machine (ALCF-3, named Aurora).

### *Argonne Tandem Linear Accelerator System (ATLAS)*

Funded by DOE/SC-NP, ATLAS 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 Californium Rare Ion Breeder Upgrade (CARIBU) 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.

### *Atmospheric Radiation Measurement Southern Great Plains (ARM-SGP) site*

Funded by DOE/SC-BER, the ARM-SGP site is the world's largest and most extensive field site for climate research. Its instruments are arrayed across 9,000 square miles, with a heavily instrumented central facility on 160 acres near Lamont, Oklahoma. In addition to operating the ARM-SGP site, Argonne oversees operations and instrumentation and provides instrument and measurement expertise to all ARM sites. Scientists from Argonne and other institutions use ARM data to advance scientific understanding of cloud, aerosol, and atmospheric processes, which supports improvements in models of the earth's climate.

### *Center for Nanoscale Materials (CNM)*

Funded by DOE/SC-BES, the CNM supports interdisciplinary nanoscience research, with an emphasis on quantum materials, manipulation of nanoscale interactions, and nanoscale dynamics. Its unique capabilities include near-field optical measurements at the extremes of space and time resolution, scanning tunneling microscopy, ultrafast electron microscopy, extreme nanofabrication, and the first generation of user tools for QIS. Collaborations with APS include a hard x-ray nanoprobe and a synchrotron x-ray scanning tunneling microscope. Significant upgrades in CNM research tools will be needed to enable the Center's users to continue making groundbreaking discoveries over the next decade. Argonne is committed to working with DOE to continue upgrading CNM instrumentation through internal investment, the CNM operating budget, and other opportunities. A recent multi-laboratory Major Items of Equipment proposal to DOE/SC-BES, for Nanoscale Science Research Centers Recapitalization, identifies opportunities to greatly strengthen our user-facility core capability.

### **Mission relevance and funding**

This 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 capabilities also is provided by DOE/NNSA, DOE/OE, NIH, NSF, and industry.

## **Nuclear and radio chemistry**

## Capability

Argonne executes pioneering work in nuclear chemical engineering, chemical separations, 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:

- Materials chemistry and thermophysical properties of actinides in extreme environments, such as the high-temperature and molten salts encountered in future nuclear energy systems
- Production and chemical separation of radioisotopes essential to groundbreaking medical and national security technologies
- Structure-property relationships foundational to 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

A distinctive portfolio of research capabilities and facilities enables this work, including:

- APS, ATLAS, and ALCF
- Electron microscopy tools including the Intermediate Voltage Electron Microscope
- Two co-located, purpose-built radiological facilities: a low-energy electron linear accelerator (LINAC) and a chemical separations system for radioisotope production and isolation
- Radiological laboratories that enable development and testing of advanced electrochemical and aqueous processes, to support development of innovative nuclear fuel cycle and safeguards technologies

We apply these capabilities to actinide science that produces novel approaches to the synthesis, characterization, and modeling of transuranic complexes. Our work uses purpose-built radiological facilities to extend understanding of the pure and applied chemistry of these artificially made elements. We target predictive bonding and energetics models, within the context of separations relevant to nuclear energy, by using Argonne computational facilities to interpret x-ray analytical characterization at the APS. We are applying the insights from these studies to develop efficient separations processes and associated safeguards technologies that promise to reduce nuclear waste generation in a secure, efficient, and cost-effective manner.

Within the context of minimizing the world's reliance on weapons-usable nuclear material in reactor applications, we are a leader in the production of molybdenum-99/technetium-99m, which is currently the most important and in demand medical isotope for diagnostic nuclear medicine. In collaboration with industrial sponsors, we have developed and demonstrated new accelerator-based production channels and chemical purification methods to facilitate domestic molybdenum -99 production without the use of weapons-usable materials.

In parallel, we are leveraging our radiochemistry expertise to develop our electron LINAC – one of the most powerful electron accelerators across the DOE complex – and radioisotope separations capability into a production facility for theranostic medical isotopes. We are poised to become a supplier of copper-67 to the DOE National Isotope Development Center (NIDC) and have ongoing radiochemistry R&D applied to other cancer-fighting medical isotopes, including scandium-47 and high-priority actinium-225. Capable of diagnosing and treating tumors such as prostate and bone cancer with targeted radiation, these radioisotopes provide a game changing approach to cancer diagnosis and treatment.

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 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 research organizations.

## **Nuclear engineering**

### **Capability**

Argonne pioneered nuclear energy systems and continues to be a world leader in advancing nuclear energy science and technology. We are recognized for ground-breaking research in both advanced nuclear energy technology and nuclear materials security. Our nuclear engineering capability supports significant national goals in nuclear power safety, nuclear energy development, nuclear nonproliferation, isotope research and production, and protection of critical infrastructure. Our nuclear engineering staff draws on unique Argonne capabilities in nuclear and neutron physics, thermal-hydraulics, materials science, nuclear and radio chemistry, 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. Using ALCF, Argonne has made groundbreaking advances in exploiting high-performance computing for multiphysics analysis of nuclear-reactor behavior. Nuclear engineering research also employs our specialized engineering development laboratories for detailed studies of nuclear reactor materials and components under prototypic conditions through the engineering scale. Throughout our history, we have enhanced the efficiency and benefits from our research through national and international collaboration with research and industrial partners.

Argonne has long invested significant effort in maintaining and expanding core capabilities in neutron physics and advanced reactor design and safety analysis. We are viewed as the world leader in designing and analyzing fast-neutron-spectrum systems and understanding the performance and safety behavior of fuels and materials in nuclear reactors. Our contributions to the design of passively safe reactor systems and our understanding of nuclear accident phenomena and mitigation are widely recognized by the international community. Building on our work with fast-spectrum reactors, we now lead the core design and safety analysis efforts for the Versatile Test Reactor, one of the priority projects of DOE's Office of Nuclear Energy.

In addition, we use our nuclear fuel cycle expertise, along with our nuclear and radio chemistry capability, to develop methods for separating radioisotopes and recycling actinides to reduce nuclear waste generation. We also have applied our understanding of reactor physics, thermal hydraulics, and materials behavior to the conversion of fuel in research and test reactors around the world from highly enriched to low-enriched uranium.

Targeted outcomes of Argonne's nuclear engineering program are:

- Leading, in partnership with Idaho National Laboratory and Oak Ridge National Laboratory, innovation in design of next-generation reactor and fuel cycle systems and development of the Versatile Test Reactor and other vital components of the national infrastructure for nuclear energy

- Increasing fundamental understanding of nuclear energy materials, processes and systems, thereby enhancing the scientific basis for their safe use and efficient regulation
- Developing and validating advanced, mechanistic modeling and simulation capabilities to improve prediction of the performance characteristics and safety behavior of nuclear energy systems
- Leading the development of the science and technology basis for limiting proliferation risk from nuclear energy systems, including minimizing the use and availability of highly enriched uranium
- Advancing the DOE/SC-NP goals for isotope production and research

### **Mission relevance and funding**

This capability supports the missions of DOE and other organizations to sustain the benefits of nuclear energy generation; develop new and innovative nuclear energy systems, including advanced testing facilities that support development of future nuclear systems; and enhance the security of nuclear technology applications worldwide. Current sponsors include DOE/ARPA-E, DOE/NE, DOE/NNSA, DOE/SC-NP, DHS, NRC, the nuclear power industry, and international organizations.

## **Nuclear physics**

### **Capability**

Argonne is a global leader in nuclear structure, nuclear astrophysics, fundamental interactions, and hadron physics as well as in the enabling areas of nuclear instrumentation and accelerator development. ATLAS remains at the cutting edge of discovery science with recent upgrades to deliver a capability set that is unique in the world. Capabilities include high-purity beams of radioactive isotopes from the Californium Rare Isotope Breeder Upgrade (CARIBU), stable beams at energies up to 20MeV/nucleon, and state-of-the-art instrumentation such as the helical orbital spectrometer (HELIOS). The recent addition of the Radioactive Ion Separator (RAISOR) further increases the availability of intense and clean light radioactive ion beams. This capability set enables Argonne staff and external ATLAS users to study nuclear structures that depend strongly on the neutron excess and are not readily apparent in stable nuclei, to investigate reactions and nuclear properties far from stability, to probe astrophysical processes generating the chemical elements, and to test nature's fundamental symmetries and interactions.

Our physicists are leaders in the theoretical and experimental study of quantum chromodynamics, the foundational force that binds protons, neutrons, and nuclei. They design, construct, and operate detectors at Thomas Jefferson National Accelerator Facility (TJNAF) and Fermilab to carry out these investigations. Argonne scientists are principal investigators for about 30% of all Jefferson Lab 12-GeV experiments. At Argonne, we test the limits of the Standard Model by searching for violation of time reversal symmetry in the electric dipole moment measurement of radium-225.

Argonne's experimental nuclear physics research is supported by our work in accelerator science and by theory efforts that make use of the ALCF and Argonne's computational capabilities. We are world leaders in quantum Monte Carlo calculations of nuclear structure and reactions and predictions of hadron and nuclear properties using nonperturbative methods in quantum chromodynamics.

We also apply our expertise to address national needs, such as characterization of spent nuclear fuel for reactor design; production techniques for medical radioisotopes in collaboration with Argonne's nuclear engineers; and atom trap trace analysis for geophysics, oceanography, and national security applications. Our one-of-a-kind national center for radio-krypton dating commenced operations in FY19. Argonne's accelerator R&D group supports ATLAS, but their expertise and facilities for cavity processing and fabrication are in high demand to support other accelerators funded by DOE/SC-NP, -HEP, and -BES: our capabilities in superconducting radiofrequency technology complement those of other national

laboratories. In FY19, for example, this support included the design and fabrication of the bunch-lengthening system for the APS Upgrade as well as the half-wave cavities and cryomodule for Fermilab's Proton Improvement Plan II project.

Ongoing upgrades to ATLAS will provide unmatched critical capabilities to complement the strengths of the Facility for Rare Isotope Beams (FRIB) when it comes online. ATLAS will remain the premier stable beam user facility, providing unique opportunities for rare isotopes research. A proposed multi-user upgrade will address user demand by simultaneously delivering two beams of different species to separate experiments; it also will enable an expanded isotope production program at ATLAS.

We continue to work with ATLAS users to identify important new capabilities, such as the neutron-generator upgrade to CARIBU and production of neutron-rich nuclei in the  $N=126$  region, essential for astrophysics and nuclear structure studies. We will continue our leadership role in the science and instrumentation at FRIB, leading the construction of the solenoidal spectrometer apparatus for reaction studies and making key contributions to instruments such as the Gamma-Ray Energy Tracking Array.

We also are developing leadership roles in new areas by leveraging our strengths in materials science, particle physics, accelerator and hard x-ray science, and advanced computing. For the proposed Electron Ion Collider (EIC), our goal is to make major contributions to the science program and the design and simulation of the detector and accelerator. Our detector R&D is aimed at bolometers and time projection chambers in support of neutrinoless double beta decay, silicon detectors for the EIC, and early-stage R&D on superconducting nanowire detectors. In QIS, our physicists will build on existing strengths in atom trapping, quantum sensors, and quantum algorithms for nuclear physics to build a strategy in collaboration with our materials and computing scientists and our CQE collaborators.

### **Mission relevance and funding**

This capability supports the DOE/SC-NP mission. Additional current sponsors include DOE/SC-BES and HEP; IAEA; DTRA-J9; NSF; and universities in the United States and abroad.

## **Particle physics**

### **Capability**

Argonne's particle physics research advances understanding of the fundamental constituents of energy and matter, the nature of space and time, and the underlying symmetries of the fundamental interactions. This work, with a record of significant contributions and leadership roles, distinguishes itself through strong collaborative efforts across Argonne and the DOE complex and with UChicago and Northwestern University.

The study of the recently discovered Higgs boson as a tool for new physics is at the center of our experimental program at the Large Hadron Collider (LHC) at CERN in Switzerland. A focused analysis program studying jets with heavy quarks is significantly advancing understanding of the role that the Higgs boson plays in nature. We are heavily involved in the design and 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 that will enable full exploration of LHC data.

The theoretical high-energy physics program at Argonne focuses on high-precision calculations of Standard Model processes, interprets experimental data in terms of physics both within and beyond the Standard Model, and makes predictions for new, well-motivated experimental searches that attempt to answer a number of open questions.

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

computing 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 ever for standard model processes, essential to the search for new physics.

Our research in theoretical and computational cosmology provides the most accurate, large-volume perspective on the dynamic evolution of the universe that is currently available. Our particle physicists, in collaboration with Argonne's computing researchers and staff from other DOE laboratories, play 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. These computational tools are run at the ALCF and other DOE leadership computing facilities; they 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, new insights into the dark sector of the universe. Our goal is to provide advanced statistical tools to the cosmology community to extract science from next-generation DOE-, NASA-, and NSF-supported surveys. Our cosmology group also leads one of the exascale computing projects funded by DOE/SC-ASCR.

Through a multidisciplinary effort, we deployed, at the South Pole Telescope, the largest focal plane to date of transition edge sensors (TES) for the third-generation experiment to detect anisotropies in the cosmic microwave background (CMB) radiation and have taken a leading role in proposing a fourth-generation, definitive, ground-based, CMB experiment. Our unique capabilities in engineering superconducting TES arrays are being used to develop ultra-sensitive sensors that could be deployed in next-generation dark matter detectors. We also will draw on existing strengths in superconducting devices for QIS, in collaborations via the CQE. We are continuing to transfer to industry our pioneering large-area photo-detectors with picosecond timing resolution and are transitioning our instrumentation program to target key challenges for the field in support of science, building on Argonne's multidisciplinary strengths.

We are playing key roles in construction of Fermilab's muon-to-electron-conversion experiment, following our completion of the most precise magnetic field map for the muon  $g-2$  experiment. We also recently provided critical engineering support for the protoDUNE long-baseline neutrino detector prototype, now deployed at CERN. Argonne was responsible for delivery of the high-voltage field cage and readout for the photodetectors; based on this work, we are exploring future roles in Fermilab's Long-Baseline Neutrino Facility/Deep Underground Neutrino Experiment (LBNF/DUNE). Argonne is responsible for delivering a half-wave cryomodule for Fermilab's Proton Improvement Plan-II project, which aims to deliver the most intense high-energy neutrino beam for LBNF/DUNE.

### **Mission relevance and funding**

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

## **Systems engineering and integration**

### **Capability**

We bring together multiple engineering disciplines to integrate science discoveries into practical technological solutions that strengthen the US energy, environmental, and security portfolio and enhance the nation's economic competitiveness. We develop experimental facilities and analytical tools to advance understanding of urban environments, communications, transportation, critical

infrastructure, and other large-scale systems. Our infrastructure work also draws on our capabilities in decision science and analysis.

For example, when Hurricane Maria struck Puerto Rico in September 2017, we deployed experts to support recovery. We provided on-the-ground infrastructure damage assessments, adapted our software tools for more-effective grid restoration, and trained local stakeholders to use those tools to better prepare the island for future storms.

As another example, we are nationally recognized for developing systems engineering methods to help overcome security, risk, resiliency, and interdependency challenges facing lifeline infrastructures. We have created tools for infrastructure analysis, design, experimentation, and computation that enable us to model the interdependencies of key systems to understand cascading effects and develop mitigations to strengthen infrastructure. 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 engineering improvements in our nation's electrical infrastructure.

Advanced computing at the ALCF is a core component of our systems engineering and integration work, including high-fidelity modeling of electric power grid systems, the mobility ecosystem, and engine combustion kinetics. In these research areas, we also apply emerging approaches, such as machine learning and artificial intelligence.

We apply the imaging capabilities of the APS to understand structure and processes in materials and chemistries, such as complex flows in engineered systems. For example, we use the APS to study fuel-injector spray dynamics and combustion chemistry in engines. This work is complemented by experiments at Argonne's Engine Research Facility, which is used to study in-cylinder combustion, fuels, and emissions under operating conditions.

We are developing a range of innovative concepts to enhance mobility through advances in areas such as autonomous vehicles; more-efficient intermodal transportation of freight; infrastructure and vehicle connectivity; and three-dimensional transportation, including electric aviation as well as unmanned and robotic mobility. With DOE/EERE support, we use our EV-Smart Grid Interoperability Center to conduct research to facilitate transatlantic interoperability between electric vehicles and their charging infrastructure, ultimately leading to smart-grid integration, grid resilience, and full infrastructure interoperability. A component of this work relies on understanding the potential for new technological paradigms enabled by discoveries in our science programs, such as concepts for advanced batteries. In this work, we draw on our expertise in vehicle energy consumption for US manufacturing job retention through our ongoing collaborations with the European Commission, industrial partners, and the United States – China Clean Energy Research Center's Clean Vehicles Consortium.

### **Mission relevance and funding**

This capability supports the missions of DOE, DHS, other federal agencies, and industry. Current DOE sponsors include DOE/EERE, DOE/NE, and DOE/OE. Current DHS sponsors include the Federal Emergency Management Agency and the Cybersecurity and Infrastructure Security Agency. Current strategic partnership sponsors include DOD, DOS, DOT, NERC, and NGA.

## Science Strategy for the Future

Argonne's strategy is grounded in the Laboratory's widely recognized leadership in taking on profound challenges in science and technology and delivering results that enable decades of further progress. Argonne's science strategy is designed to produce game-changing advances in both fundamental and applied research:

- The world's leading hard x-ray microscope – the upgraded Advanced Photon Source (APS)

- The nation’s first exascale computer, Aurora, in the Argonne Leadership Computing Facility (ALCF)
- Cosmology and nuclear physics discoveries that illuminate long-standing mysteries of physical science
- Establishment of the basic scientific principles of multiscale assembly of functional matter
- Breakthroughs in scale-up and process technologies for manufacturing advanced materials
- New materials, devices, and software for quantum information science (QIS)
- Artificial intelligence (AI) approaches that transform the speed of scientific research

Argonne’s exceptional research staff, powerful experimental tools and facilities, and rich network of external partners provide a broad foundation for our strategy. In addition, UChicago supports Argonne’s goals through enterprise-level partnerships, most notably:

- Center for Molecular Engineering (CME), based at Argonne and established in 2019 as a partner to UChicago’s Pritzker School of Molecular Engineering. Both the Center and the School grew out of the joint UChicago-Argonne Institute for Molecular Engineering formed in 2011. Through CME, Argonne and UChicago researchers jointly translate advances in materials science, physics, chemistry, biology and computation into new tools to address important societal problems.
- Chicago Quantum Exchange (CQE), formed in 2017 as an intellectual hub to advance QIS; the CQE is anchored by UChicago, Argonne, Fermilab, and the University of Illinois at Urbana-Champaign. It also includes the University of Wisconsin at Madison, Northwestern University, and six corporate partners.
- Joint Task Force Initiative (JTFI), launched in 2018 with Fermilab, to drive development of high-impact research programs drawing on the combined strengths of the three organizations
- Argonne@Chicago, a potential second location for Argonne staff on the UChicago campus, now in conceptual development, to strengthen local collaborations and support Chicago’s growth as an innovation economy

We are pursuing our strategic goals through the major initiatives and emerging initiatives described below, to unlock new frontiers in science and technology.

## Infrastructure

### Overview of Site Facilities and Infrastructure

Argonne’s site in suburban Chicago is overseen by DOE/SC. The average age of Argonne-operated facilities and infrastructure is 48 years, with 61% of the assets being more than 50 years old. Our facilities are roughly 90% occupied.

In addition to buildings operated by Argonne, the site includes the Howard T. Ricketts Regional Biocontainment Laboratory, operated by UChicago, and the Theory and Computing Sciences Building, a privately-operated building in which we currently rent about 240,000 sq ft.

In December 2018, a new lease agreement was signed for 30,000 sq ft of data center space at the Theory and Computing Sciences Building. When occupied, this new space will support exascale computing in addition to Argonne’s advanced computing initiative. In FY19, we plan to lease 60,000-80,000 sq ft of multi-use space in support of the APS-U project.

### Campus Strategy

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. The plan prioritizes needs, with timing and sequencing of actions chosen to align with the mission and leverage resources available for execution. 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, improving asset condition, 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 utility infrastructure. We use a rigorous process to assess site infrastructure conditions to prioritize and implement repairs and upgrades to meet capacity, reliability, and redundancy goals. The goal of our planned investments is to reduce our identified deferred maintenance backlog, with an ultimate target of achieving the DOE-established goal for “adequate” condition for all utility infrastructure.
- Address legacy waste and excess facilities. Removal of legacy waste and excess facilities is consistent with the DOE/SC goal of maximizing asset utilization and eliminating inadequate-condition facilities. It also supports complex-wide DOE requirements for overall footprint reductions via space banking and reduction in yearly operations and maintenance costs. We are aggressively consolidating radiological facilities and reducing inventories of radiological materials, while preserving the capability to perform mission-important activities. The biggest challenge in this area is securing external funding for disposition of contaminated facilities. As part of the FY20-FY24 DOE/EM budget call, Argonne submitted a five-year over-target request of \$143 million with 14 subproject activities. Execution of the excess facilities strategy in the identified period is critical to the Laboratory’s long-term deferred maintenance reduction and facility utilization strategy. Argonne will continue to work in close coordination with DOE/SC to obtain the needed funding and is prepared to respond to DOE/EM’s FY20-FY24 budget call if invited to do so.

Key near-term investments to achieve Argonne’s infrastructure strategy:

- *Materials Design Laboratory (\$95 million SLI)*. Now under construction, the Materials Design Laboratory is on track for beneficial occupancy in FY19 within cost, scope, and schedule. This 115,000-sq-ft facility will enable continued consolidation of research space that began with the Energy Sciences Building, to support three 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.
- *Electrical capacity distribution capability (\$60 million SLI)*. An upgrade to Argonne’s high-voltage power supply is required to support projected load increases associated with scientific growth and provide a fully redundant power supply to all site research programs, facilities, and systems. Argonne today receives power from a single location that has original 1960 equipment and installations. This condition increases the risk of an external power outage affecting the site and mission-critical programs, including the Advanced Photon Source (APS), Center for Nanoscale Materials (CNM), Argonne Leadership Computing Facility (ALCF), and Argonne Tandem Linear Accelerator System (ATLAS). The power upgrade also will provide additional capacity to support

increases in electrical usage associated with exascale computing efforts expected in the FY21 timeframe. This investment is considered enabling infrastructure; however, it directly addresses risks associated with the following core capabilities: accelerator science and technology; advanced computer science, visualization and data; chemical and molecular science; condensed matter physics and materials science; and nuclear physics.

- *Major utilities repair and modernization (\$90 million SLI)*. This project replaces, repairs, and upgrades several critical utility systems (chilled water, domestic water, steam/condensate, and sewer) to reduce operational risks, eliminate deferred maintenance, and reduce the risk of unplanned service outages. Upgrades to central chilled water capacity and distribution will enable integration of isolated buildings, reducing operating and maintenance costs and decommissioning aging satellite plants and associated failing equipment. Repairs and replacements will address deteriorated and failed portions of steam and condensate distribution piping. The project also will replace an obsolete, unsupported control system for the steam plant. This investment is considered enabling infrastructure; however, it directly addresses risks associated with the following core capabilities: accelerator science and technology; advanced computer science, visualization and data; chemical and molecular science; condensed matter physics and materials science; and nuclear physics.
- *400-area facility, modernization (mechanical \$7.1 million GPP, electrical \$8.4 million GPP)*. Multiple investments are required to modernize the 400 area of the site to assure that several mission-critical facilities – APS, CNM and the Advanced Protein Characterization Facility (APCF) – can continue to function as 24/7 scientific user facilities. The main support facilities and utility distribution are original, installed approximately 26 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 general facility roof replacements. Direct funding is required to replace the primary support cooling systems and the underground piping and electrical distribution. This investment primarily supports the following core capabilities: accelerator science and technology, biological and bioprocess engineering, chemical and molecular science, condensed matter physics and materials science, and large-scale user facilities/advanced instrumentation.
- *Building 350 legacy project and renovation (\$44.1 million SLI, \$8.9 million 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 21,000 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, safety, and health support operations.

### **Alternative financing approaches**

Argonne continues to investigate alternative financing approaches to achieving the site's facilities modernization strategy. Through partnerships with the State of Illinois, Argonne has constructed several facilities, most recently the APCF.

To address future growth in several areas – energy storage, imaging, microscopy, and materials synthesis scale-up – we have proposed the Illinois Energy Storage Accelerator building (formerly known as the Energy Innovation Center), the Sensing and Imaging at Argonne building, and the Materials Scale-up Laboratory (formerly known as the Applied Materials Manufacturing Facility).

## Site Sustainability Plan Summary

Argonne's site sustainability program supports our science and engineering mission by modernizing infrastructure and engaging site occupants while reducing Argonne's environmental impact. We have made sustainability improvements under four active energy savings performance contracts (ESPCs) and are now measuring the results. Improvements include the Combined Heat and Power Plant and efficiency upgrades in boiler house operations, site lighting, and building controls. We continue to participate in the DOE Facilities and Infrastructure Restoration and Modernization Program and have hosted experts from the Federal Energy Management Program to learn about implementing energy efficiency projects through a utility energy service contract (UESC).

In FY18, our sustainability accomplishments included completion of 23 energy and water efficiency projects, which provide \$170,000 in annual savings to the Laboratory, and installation of an additional 40 kW of solar photovoltaics at Bldg. 300. In the second year of our Retrocommissioning (RCx) Program, our RCx contractor completed analysis and testing at Bldgs. 201, 208, 221, and 362 and recommended measures that will deliver \$147,000 in annual savings to Argonne. We are incorporating RCx strategies specific to sustainable experimental laboratories through participation in the DOE Smart Labs Accelerator (SLA). We joined the SLA in FY18 and now are collaborating with partners to implement best practices to enhance safety and energy efficiency.

In July 2018, Argonne implemented a composting program that focuses on food scraps and paper towels and so far, has collected five tons of material monthly. We have documented 16 buildings as meeting High-Performance Sustainable Buildings Guiding Principles, meeting DOE's goal of 17% by FY25.