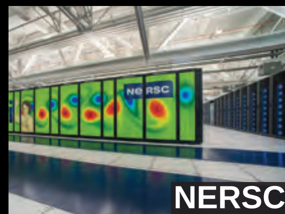
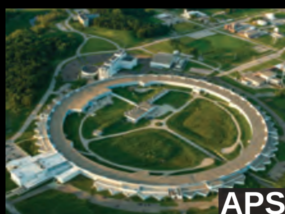
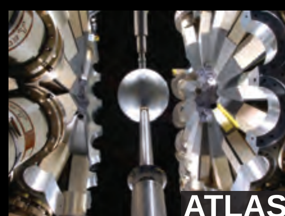
Science Day Program

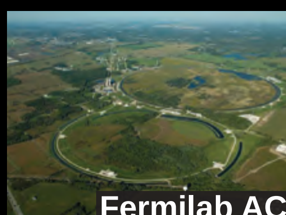
April 26, 2019

27 scientific
user facilities
35,000 users









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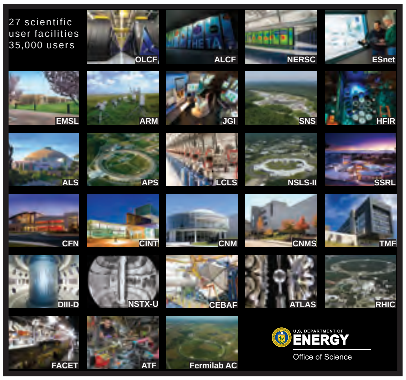

On the cover:

A pictorial collage depicting the Office of Science's 27 state-of-the-art national scientific user facilities, comprising the most advanced tools of modern science, helping researchers propel the U.S. to the forefront of science, technology development, and deployment through innovation.

Scientific User Facilities

One of the DOE Office of Science's (SC) most important contributions to the U.S. scientific effort is support of the construction and operation of major scientific user facilities at the DOE national laboratories. This was intended to be an integral part of the DOE national laboratories' mission from the start. One purpose of the national laboratories, when they were first established after World War II, was to serve as home to large, costly scientific facilities that universities could not afford but that would be essential for America to maintain leadership in science. SC user facilities are now defined as federally sponsored research capabilities available for external use to advance scientific or technical knowledge under the following conditions:

- The facility is open to all interested potential users without regard to nationality or institutional affiliation.
- Allocation of facility resources is determined by merit review of the proposed work.
- User fees are not charged for non-proprietary work if the user intends to publish the research results in the open literature. Full cost recovery is required for proprietary work.
- The facility provides resources sufficient for users to conduct work safely and efficiently.
- The facility supports a formal user organization to represent the users and facilitate sharing of information, forming collaborations, and organizing research efforts among users.
- The facility capability does not compete with an available private sector capability.

There are 27 DOE Office of Science user facilities, with all but one located at DOE national laboratories. Each year more than 35,000 researchers make use of these facilities, with access determined on a competitive basis using peer review. The decision to invest in a user facility emerges through long term strategic planning with the scientific community to identify the research tools that will deliver the greatest scientific impact to advance the DOE mission. Successfully building these facilities relies upon SC's strong culture of project management.

Each user facility represents a substantial commitment on the part of its sponsoring SC research program office, which provides oversight and works closely with the facility management to maximize scientific impact and productivity. These large-scale facilities have become increasing vital in certain key areas of research, especially areas with major potential impact on industrial innovation and national economic competitiveness. As a result, the global competition in certain categories of facilities has grown increasingly fierce in recent years.

Dr. Patricia Dehmer, this year's Science Day Plenary speaker, will introduce this topic to you. Dr. Dehmer's talk will be followed by presentations highlighting a sample of SC's user facility portfolio, including an introduction to project management, research at the Center for Integrated Nanotechnologies (CINT), the Linac Coherent Light Source (LCLS), and the Advanced Photon Source (APS), and a tutorial on accelerator science and technology, which is at the heart of numerous facilities.

Key SC user facilities include:

- *Supercomputers.* Supercomputers have become enormously powerful tools of both science and industry—enabling modeling and simulation of complex systems beyond the reach of experiment and accelerating the process of industrial design of such major items as jet turbines and fuel-efficient vehicles. DOE leads the U.S. supercomputing effort, with the DOE Office of Science spearheading high performance computing for open science and industry, at the Argonne and Oak Ridge Leadership Computing Facilities and the National Energy Research Scientific Computing Center at Lawrence Berkeley National Laboratory (LBNL). Currently, DOE owns the world's fastest supercomputer, Summit at Oak Ridge National Laboratory (ORNL), and five out of the world's fastest ten. But it will require sustained effort to ensure continued leadership as other nations continue to race ahead with new deployments.
- *X-Ray Light Sources.* X-ray light sources are critical tools for materials science, chemistry, and biology, as well as powerful instruments for medical research and pharmaceutical discovery. The DOE Office of Science fields five of these: the Linac Coherent Light Source (LCLS) and Stanford Synchrotron Radiation Lightsource (SSRL); the Advanced Photon Source (APS); the Advance Light Source (ALS); and the National Synchrotron Light Source-II (NSLS-II). The LCLS is the world's first hard x-ray free electron laser facility capable of producing x-rays that are both very intense and clumped into ultrafast pulses, while the other four light sources are synchrotrons, each with defining characteristics. The SSRL produces intense x-rays as a resource for researchers to study our world at the atomic and molecular level, allowing for research and

advances in energy production, environmental remediation, nanotechnology, new materials and medicine; the APS is one of only four third-generation, hard x-ray synchrotron radiation light sources in the world; the ALS is one of the world's brightest sources of high-quality, reliable vacuum-ultraviolet light and soft X-rays, enabling a wide variety of scientific disciplines enabling new discoveries in a wide range of scientific fields; and the NSLS-II is a state-of-the-art synchrotron light source which allows for scientists to probe the fundamental properties of matter, paving the way to new scientific discoveries and innovations. The U.S. once commanded the light source landscape, but international competition has intensified, which also explains why four out of the five DOE light sources are at one stage or another of upgrade to maintain U.S. preeminence in this area.

- *Neutron Scattering Sources.* Neutrons provide an alternative window into matter and have similarly important applications to materials, chemistry, and biology. The DOE Office of Science has two such facilities at ORNL—the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR). SNS is in the early stages of adding a second target station.
- *Nanoscale Science Research Centers.* Nanoscience, the investigations of matter on the scale of a nanometer, or 1 billionth of a meter, 1/100,000 the width of a human hair, has become key to innovation in energy and a range of other industrial applications. The DOE Office of Science operates five such centers with specialized equipment at Argonne, Brookhaven, Oak Ridge, Lawrence Berkeley, and one co-located at Los Alamos and Sandia National Laboratories, accessed by thousands of users from universities, national laboratories, and other institutions across the country each year.
- *Biological and Environmental Facilities.* Genomics has become increasing vital as we move toward a new bio-economy with expanding production of fuels and products from reengineered microbes and renewable plant resources. The Joint Genome Institute (JGI) is the world's largest sequencing center for microbes and plants related to energy and environment, has thousands of users nationwide, and sequences 200 trillion base pairs per year. The Atmospheric Radiation Measurement (ARM) user facility is a multi-platform scientific user facility with instruments at fixed and varying locations around the globe for obtaining continuous field measurements of atmospheric data. The Environmental Molecular Sciences Laboratory (EMSL) provides the scientific community with a problem-solving environment that enables researchers to use multiple combinations of capabilities to obtain a mechanistic understanding of physical, chemical, and intra- and inter-cellular processes and interactions, and to incorporate this information into numerical models to better understand how biological, environmental, atmospheric, and energy systems function at higher spatial- and temporal scales, and to address complex challenges facing DOE and the nation.
- *Fusion and Plasma Sciences Facilities.* DIII-D National Fusion Facility (DIII-D), the largest magnetic fusion user facility in the U.S., is a tokamak confinement device with significant engineering flexibility to explore the optimization of the advanced tokamak approach to fusion energy production. The National Spherical Torus Experiment – Upgrade (NSTX-U) is a magnetic confinement fusion facility employing a spherical torus confinement configuration to explore the potential stability and confinement advantages of this compact tokamak concept.
- *High Energy Physics and Accelerator Science.* The Fermilab Accelerator Complex consists of four accelerators that work together to provide world-class particle beams for experiments at the Intensity Frontier. The Facility for Advanced Accelerator Experimental Tests (FACET) is an Accelerator-based User Facility where experiments in beam-driven plasma wakefield particle acceleration are carried out. The Accelerator Test Facility (ATF) provides users with high power lasers synchronized with high brightness electron beams, providing a testbed for exploring the science of particle acceleration and radiation generation, and for developing new accelerator technologies.
- *Nuclear Physics.* The Argonne Tandem Linac Accelerator System (ATLAS) is a leading facility for nuclear structure research in the United States providing a wide range of beams for nuclear reaction and structure research to a large community of users from the US and abroad. The Relativistic Heavy Ion Collider (RHIC) is a world-class scientific research facility which hundreds of physicists from around the world use to study what the universe may have looked like in the first few moments after its creation. The Continuous Electron Beam Accelerator Facility (CEBAF) is a world-leading facility in the experimental study of hadronic matter, used by scientists to probe the interior of the nucleus to study its properties.

More information on DOE Office of Science user facilities can be found at https://science.energy.gov/user-facilities/.

About the Sessions

All participants will enjoy the Plenary Session in the Aiton Auditorium. For Seminar Sessions I and II, students can choose to attend the session that interests them the most. Make sure to get to the sessions on time as the seats fill up fast! All of the speakers are presenting during both sessions, so once all of the seats are filled in a room, participants will be asked to attend a different presentation for that seminar block.

Sessions by Times and Locations

PLENARY SESSION: 8:20 – 9:45 a.m.

Room	Title / Speaker	Page
Aiton Auditorium	The Scientific User Facilities in DOE's Office of Science – 21st Century Tools of Science - Dr. Patricia Dehmer	4

SEMINAR SESSION I: 10:00 – 11:15 a.m.

Room	Title / Speaker	Page
Ohio Room	Next Steps and Challenges in Translating Nanoscience into Nanotechnology - Dr. Millicent (Millie) Firestone	5
Clover Room	Lights, Camera, Action! Catching Atomic Motion in the Act with the World's First X-ray Free Electron Laser - Dr. James Glownia	6
Iowa Room	Synchrotron X-ray Snapshots of Molecules in Motion - Dr. Anne Marie March	7
America Room	Particle Accelerators: Science, Technology, and Applications - Dr. Todd Satogata	8
Missouri Room	Constructing Large Cutting-Edge Science Projects - Mr. Jeffrey Sims	9

SEMINAR SESSION II: 1:00 – 2:15 p.m.

Room	Title / Speaker	Page
Ohio Room	Next Steps and Challenges in Translating Nanoscience into Nanotechnology - Dr. Millicent (Millie) Firestone	5
Clover Room	Lights, Camera, Action! Catching Atomic Motion in the Act with the World's First X-ray Free Electron Laser - Dr. James Glownia	6
Iowa Room	Synchrotron X-ray Snapshots of Molecules in Motion - Dr. Anne Marie March	7
America Room	Particle Accelerators: Science, Technology, and Applications - Dr. Todd Satogata	8
Missouri Room	Constructing Large Cutting-Edge Science Projects - Mr. Jeffrey Sims	9

Dr. Patricia Dehmer
Plenary Session
Aiton Auditorium
8:20 – 9:45 a.m.

The Scientific User Facilities in DOE's Office of Science – 21st Century Tools of Science

The scientific user facilities are an iconic component of DOE's Office of Science (SC) portfolio. They enable researchers to explore and model the universe—from the subatomic world, to the familiar world of everyday materials and chemicals, to the farthest reaches of the cosmos. They drive fundamental scientific discoveries; assist industry with new materials development, improved manufacturing processes, and advanced product testing; and help ensure our national and economic security. They attract tens of thousands of researchers from around the world each year, and they enable discoveries that change the course of science. This year, more than 36,000 researchers from universities, national laboratories, industry, and international institutions will use the 27 SC scientific user facilities. Nobel prizes in disciplines ranging from particle physics to molecular biochemistry have been awarded for research performed at these facilities over the decades of their existence. Usually large and costly to build and operate, these facilities require substantial resource commitments. The planning process for the largest of the facilities—those in the billion-dollar range—often extends over many years and involves hundreds, sometimes thousands, of potential users. The facilities are open to all with access determined solely by merit review of proposed work and are available at no charge for nonproprietary work. Maintaining the existing scientific user facilities and constructing new ones are among the most important activities of SC and its system of laboratories. Today, the budget for operating and constructing the scientific user facilities is more than half that of the entire Office of Science, which is $6.58 billion in FY 2019. These facilities, together with the attendant concept of "big science," helped define the nature the Office of Science portfolio and those of the 17 DOE national laboratories.

About the Speaker:

Dr. Patricia Dehmer is the former Deputy Director for Science Programs in the Office of Science (SC) in the U.S. Department of Energy (DOE) and the former Director of the Office of Basic Energy Sciences (BES) within SC. As the Deputy Director, she was the senior career science official in SC and was the Acting Director between Senate-confirmed Presidential appointees. As Director of the BES Program, she was known for her broad support of physical science research and for the planning, design, and construction phases of a dozen major scientific construction projects totaling more than $3 billion. Notable were the $1.4 billion Spallation Neutron Source at Oak Ridge National Laboratory; five Nanoscale Science Research Centers totaling more than $300 million; and two facilities for x-ray scattering, each in the billion-dollar range — the Linac Coherent Light Source at SLAC, which is the world's first hard X-ray free electron laser, and the National Synchrotron Light Source II at Brookhaven National Laboratory. During her federal service, Dr. Dehmer was awarded the James R. Schlesinger Award – the highest recognition in DOE – for management of SC's portfolio in the physical sciences and for outstanding management of the Department of Energy's largest-scale scientific construction projects. Previously, Dr. Dehmer was a Distinguished Fellow at Argonne National Laboratory with research activities in atomic, molecular, optical, and chemical physics. Since her retirement from federal service in late 2016, Dr. Dehmer works as a management consultant with additional service on boards, science advisory committees, and professional society committees. She is a fellow of the American Physical Society and the American Association for the Advancement of Science.

Dr. Millicent (Millie) Firestone
Ohio Room
10:15 – 11:30 a.m.
1:00 – 2:15 p.m.

Next Steps and Challenges in Translating Nanoscience into Nanotechnology

Mastering control over the assembly of nanoscale building blocks to form complex functional materials is a fundamental tenet of nanoscience. Approaches to the preparation of nanoscale materials are diverse, and include the construction of nanoparticle superlattices by surface functionalization to achieve precise control over inter-particle spacing and crystal habits or the use of lithographic patterned surfaces for directed nanoparticle organization. Each of the aforementioned strategies for nanomaterial preparations, however, is cost ineffective due to a reliance on expensive components or instrumentation, lack of scalability, and a failure to yield bulk processable materials amenable to high throughput nanomanufacturing. These factors are essential for effective translation of nanoscience into nanotechnology. An alternative tactic for nanomaterials construction, that addresses the noted limitations, is the creation of nanoparticle polymer composites prepared by bottom-up self-assembly of custom designed molecular monomers to form liquid crystals that can be subsequently captured as durable, elastic materials by polymerization. In this presentation, I will discuss a versatile bottom-up, self-assembly synthetic procedure for the formation of nanoparticle polymer composites that integrate and geometrically organize a wide variety of nanoparticles within a structured matrix, giving rise to both synergistic and emergent properties. The coupling of top-down 3D-printing with bottom-up self-assembly is further used to promote integration across length scales, spanning nanoscale to microscale. The benefits of achieving nano to system level integration will be discussed in the context of fabricating flexible nanoelectronics and nanophotonics. Work solving the challenge of accurate structural characterization/metrology of these multicomponent, hierarchically structured composites through X-ray scattering by employing the capabilities at the DOE light sources will also be highlighted.

About the Speaker:

Dr. Millicent (Millie) Firestone received her Ph.D. in chemistry from Northwestern University in Evanston, IL. After post-doctoral work at the University of Illinois Urbana-Champaign, she joined Argonne National Laboratory (Lemont, IL) where she led a program in biomolecular materials for more than 13 years. In 2013, Los Alamos National Laboratory recruited Millie as a strategic hire to lead the soft matter effort at the Center for Integrated Nanotechnologies in the Materials Physics and Applications Division. Currently, Millie is working to bridge basic nanoscience efforts with mission work at Los Alamos. She was one member of a large multidisciplinary team recognized for these efforts by being awarded a NNSA Defense Program Award for significant contributions to stockpile stewardship. Dr. Firestone has published over 100 referred publications in the fields of soft materials, X-ray and neutron scattering, and synthesis of nanocarbons under extreme conditions.

Dr. James Glownia
Clover Room
10:15 – 11:30 a.m.
1:00 – 2:15 p.m.

Lights, Camera, Action! Catching Atomic Motion in the Act with the World's First X-ray Free Electron Laser

The text you are reading in this abstract may look stationary, but all of the electrons, atoms, and molecules that comprise it are always in motion. This is due to the laws of quantum mechanics, and on the microscopic length and time scale nothing is ever truly at rest. These tiny motions are responsible for keeping us warm, for allowing plants to collect sunlight, for the electronics in your smart phone to function, chemical reactions, etc. Until fairly recently this motion has been too fast to observe even with the most powerful electron microscopes. At the SLAC National Accelerator lab we have developed the Linac Coherent Light Source, which is a mile long electron particle accelerator based laser that can generate flashes of x-ray laser light on the femtosecond (10-15 s) or 1 millionth of a billionth of a second. These flashes are bright, short, and small wavelength enough to effectively freeze atomic and molecular motion. In this talk, I will describe how this laser works and show how we utilize these individual snapshots to make molecular movies. I will also describe a few of the interesting problems we have studied such as chemical reactions that are responsible for your vision, the steps involved in photosynthesis, magnetic spins in materials, and matter in the center of stars. Lastly, I will discuss my role as a scientist at this unique facility, where I generally interact with hundreds of other scientists a year to conduct collaborative research.

About the Speaker:

James Glownia is a staff scientist at the SLAC National Accelerator Lab working at the Linac Coherent Light Source (LCLS). Much of his work focuses on developing and implementing new femtosecond optical laser sources and techniques for use with LCLS. These sources are used in conjunction with the x-rays from LCLS to observe motion on the angstrom length scale and femtosecond time scale. He is also on the x-ray beamline support staff where he is part of the teams that execute user proposed experiments at LCLS to take advantage of its unique capabilities. His own scientific research is focused around using x-rays to create movies of molecules undergoing an optical laser induced chemical reaction, and on finding ways to get interesting physical or chemical insight out of these movies. In particular, he has been able to make the first true de-novo images of molecular vibrations and is currently working on observing and understanding the simultaneous flow of energy on multiple levels of an excited molecule. He received a Ph.D. in applied physics from Stanford University and a B.S.E in engineering physics from the University of Michigan.

Dr. Anne Marie March
America Room
10:15 – 11:30 a.m.
1:00 – 2:15 p.m.

Synchrotron X-ray Snapshots of Molecules in Motion

Synchrotron X-ray facilities are arguably the most powerful tools invented for understanding the structure of matter at the atomic scale. They produce bright beams of X-rays that can penetrate materials, providing insight into otherwise hidden interior structure. The bright beams can yield information about the elemental composition of materials due to the fact that each element of the periodic table has characteristic X-ray absorption energies. And because the wavelengths of X-rays are very small, on the same order as atomic distances in materials (ranging from about 0.01 nanometers to 10 nanometers), they allow us to see extremely small structures, all the way down to the level of individual atoms.

The Advanced Photon Source (APS) at Argonne National Laboratory, outside Chicago, IL, is one of five X-ray light sources in the U.S. operated by the Department of Energy and one of only four so-called third-generation synchrotron light sources in the world providing very high energy X-rays. The X-rays at the APS are one hundred billion times brighter than the X-rays produced by medical X-ray machines and the experiments carried out at the APS span nearly every scientific discipline. In this talk I'll describe the three main classes of measurements that are used to "see" the structure of materials: imaging, scattering, and spectroscopy. I'll also, then, describe my own scientific studies at the APS using time-resolved hard X-ray spectroscopy techniques to see structural changes that occur as molecules react on the ultrashort picosecond (10-12 seconds) timescale.

About the Speaker:

Anne Marie March is a physicist in the Chemical Sciences and Engineering Division at Argonne National Lab. She works on advancing new time-resolved X-ray probes of molecules in solution to understand how energy flow and solvent dynamics affect chemical reactivity. She joined Argonne in 2009 as a postdoctoral researcher. She earned her Ph.D. from Stony Book University, investigating the physics of atoms in ultrashort, intense, mid-infrared laser fields and a B. A. in physics from the College of the Holy Cross.

Dr. Todd Satogata
America Room
10:15 – 11:30 a.m.
1:00 – 2:15 p.m.

Particle Accelerators: Science, Technology, and Applications

Particle accelerators are best known for their use in high energy and nuclear physics. They are the tools that have been used to discover almost all fundamental subatomic particles and study their properties, culminating with the discovery of the Higgs particle in LHC experiments earlier this decade. The highest energy beams are also the most precise demonstrations of special relativity ever created. Accelerator technology applies the latest advances in materials science such as high-field superconductors and nanotechnology. Accelerators, and the beams they produce, are also used in nearly every science discipline, with applications in biology, medicine, chemistry, and even nanotechnology.

In this talk, Dr. Satogata will introduce the discipline of accelerator physics, the study of the science of particle accelerators, and how we control, measure, and use the beams that they produce. We will explore the technology of particle accelerators, and how physicists are working with modern laser and plasma technology to bring forth the next generation of more compact accelerators. We will also survey the broad range and impacts of accelerator technology, from free-electron laser imaging that can take movies of chemical reactions and image proteins, to proton radiotherapy that is used to cure cancers, to their surprisingly most common use -- the beam business of industrial applications, including environmental remediation and clean energy production.

About the Speaker:

Todd Satogata is Director of the Center for Advanced Studies of Accelerators at Jefferson Lab, and a Jefferson Lab Professor at the Center for Accelerator Science at Old Dominion University. During his career, he has worked on the design, construction, commissioning, and operations of the Relativistic Heavy Ion Collider at Brookhaven National Laboratory (BNL), commissioning and operations of the 12 GeV CEBAF upgrade at Jefferson Lab, and design of the next-generation U.S. Electron-Ion Collider. He has made contributions to collider design and operations, medical accelerator design, proton beam imaging techniques, accelerator control systems, and broader accelerator science publication and outreach. He is co-author, with Stephen Peggs (BNL), of the recent Cambridge University Press textbook, “Introduction to Accelerator Dynamics.” He earned a Ph.D. in physics and astronomy from Northwestern University in 1993, and B.S. (physics) and B.A. (mathematics) degrees from the University of Cincinnati in 1987.

Mr. Jeffrey Sims
Missouri Room
10:15 – 11:30 a.m.
1:00 – 2:15 p.m.

Constructing Large Cutting-Edge Science Projects

Delivering large complex projects involves bringing together a team of experienced professionals, focusing them on a common goal and putting in place rigorous processes to ensure the project is completed safely, on time and within budget. This presentation will provide background on the SLAC National Accelerator Laboratory, its mission and will discuss an ongoing megaproject, the Linac Coherent Light Source II, a superconducting x-ray free electron laser that will begin operation in 2021. In addition, the talk will consider three essential tools used to lead large complex projects including their applicability to our every day lives.

About the Speaker:
Jeff Sims has 30 years of project management, engineering and construction experience on large complex science facilities including 21 years at three DOE national laboratories (SLAC National Accelerator Laboratory, Argonne National Laboratory and Fermi National Laboratory). He has lead $2B complex cutting-edge research-related projects including the $1B Linac Coherent Light Source II project which is a superconducting X-ray free electron laser under construction at SLAC National Accelerator Laboratory. Mr. Sims is also the Director of DOEs Project Leadership Institute which in a partnership with Stanford University develops project leaders across the DOE complex through a combination of experiential training and graduate level coursework. Jeff has a Bachelor’s Degree in structural engineering and is a licensed professional engineer, licensed structural engineer and a certified project management professional.

About the Office of Science

The Office of Science's (SC) mission is to deliver scientific discoveries and major scientific tools to transform our understanding of nature and advance the energy, economic and national security of the United States. SC is the Nation's largest Federal sponsor of basic research in the physical sciences and the lead Federal agency supporting fundamental scientific research for our Nation's energy future. SC accomplishes its mission and advances national goals by supporting:

- *The frontiers of science — exploring nature's mysteries from the study of fundamental subatomic particles, atoms, and molecules that are the building blocks of the materials of our universe and everything in it to the DNA, proteins, and cells that are the building blocks of life. Each of the programs in SC supports research probing the most fundamental disciplinary questions.*

- *The 21st Century tools of science — providing the nation's researchers with 27 state-of-the-art national scientific user facilities - the most advanced tools of modern science - propelling the U.S. to the forefront of science, technology development, and deployment through innovation.*

- *Science for energy and the environment — paving the knowledge foundation to spur discoveries and innovations for advancing the Department's mission in energy and environment.*

SC supports a wide range of funding modalities from single principal investigators to large team-based activities to engage in fundamental research on energy production, conversion, storage, transmission, and use, and on our understanding of the earth systems. SC is an established leader of the U.S. scientific discovery and innovation enterprise. Over the decades, SC investments and accomplishments in basic research and enabling research capabilities have provided the foundations for new technologies, businesses, and industries, making significant contributions to our nation's economy, national security, and quality of life.

Acknowledgments

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