QUADRENNIAL TECHNOLOGY REVIEW

AN ASSESSMENT OF ENERGY TECHNOLOGIES AND RESEARCH OPPORTUNITIES

DEPARTMENT OF ENERGY
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Chapter 9: Enabling Capabilities for Science and Energy
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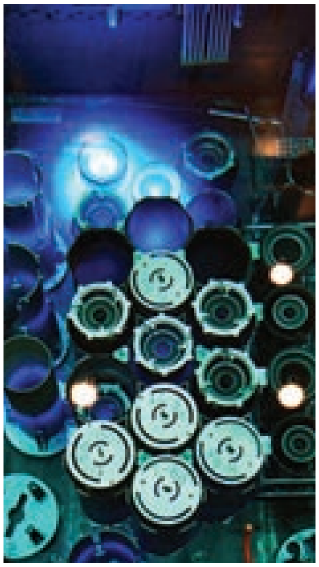


Tools for Scientific Discovery and Technology Development

- Investment in basic science research is expanding our understanding of how structure leads to function—from the atomic- and nanoscale to the mesoscale and beyond—in natural systems, and is enabling a transformation from observation to control and design of new systems with properties tailored to meet the requirements of the next generation of energy technologies.
- At the core of this new paradigm is a suite of experimental and computational tools that enable researchers to probe and manipulate matter at unprecedented resolution. The planning and development of these tools is rooted in basic science, but they are critically important for technology development, enabling discoveries that can lead to broad implementation.
- These tools are available through a user facility model that provides merit-based open access for nonproprietary research. Each year, thousands of users leverage the capabilities and staff expertise for their research, while the facilities leverage user expertise toward maintenance, development, and application of the tools in support of the broader community of users.
- The challenges in energy science and technology development increasingly necessitate interdisciplinary collaboration. The multidisciplinary and multi-institutional research centers supported by DOE are designed to integrate basic science and applied research to accelerate development of new and transformative energy technologies.
- Capabilities supported by DOE and the DOE-Office of Science (SC) are enabling the following across science and technology:
  - The X-ray light and neutron sources provide unprecedented access to the structure and dynamics of materials and the molecular-scale basis of chemical reactions. These tools, combined with novel nanoscale synthesis and fabrication techniques, are being used to develop a new era of control science at the mesoscale that will lead to novel materials for energy applications, including batteries, photovoltaics, and catalysts.
  - New technologies for energy and environmental applications based on or inspired by biological systems are enabled by advances in genomic, analytical, and observation tools. These developments are leading to designer plants for biofuel production and new climate models that produce more accurate forecasts for future energy needs.
  - Modeling, simulation, and data analysis using high-performance computers offers researchers the opportunity to simulate complex real-world phenomena, interpret large data sets, and accelerate development of new technology. The next generation of hardware, software, and algorithms offers the opportunity to computationally design complex systems for energy and environmental applications.
- Analysis of the research and development opportunities across the six energy technology chapters shows a crosscutting need for new materials and modeling, simulation, and data analytics. Careful and ongoing strategic planning by DOE-SC supports both of these scientific themes.

9

Enabling Capabilities for Science and Energy

Basic science, including the tools needed to facilitate discovery, expands our understanding of the natural world and forms the foundation for future technology. The current imperative—energy systems that meet our energy security, economic, and environmental challenges—requires advances in energy generation, storage, efficiency, and security that demand a new generation of materials (including biological and bio-inspired materials) that may not be naturally available. However, creating these new materials requires a level of understanding of the relationships between structure and function, and across many spatial scales, which is not yet supported by our understanding of the physical world. Basic scientific research is necessary to fill these knowledge gaps and enable creation of new materials with the specific characteristics needed for next-generation energy technology.

As described in the 2004 National Nanotechnology Initiative[1] workshop report, *Nanoscience Research for Energy Needs*,[2] all elementary steps of energy conversion take place at the atomic and nanoscale. The ability to rationally tailor matter at such scale would enable production of new materials for energy applications, including photovoltaics, electrodes and electrolytes, smart membranes, separators, superconductors, catalysts, fuels, sensors, and piezoelectrics. By extension, tailoring biological materials—from microbes to plants—at the genomic and sub-cellular levels would enable more efficient means of conversion, including those required to produce renewable and sustainable biofuels and bioproducts.

The current challenge in materials science is to understand how nanoscale phenomena translate to properties at the mesoscale and beyond. Quantum mechanics describes atomic, molecular, and nanoscale phenomena, while classical mechanics describes macroscale behavior. The organizing principles governing emergent phenomena at the mesoscale, where classical properties first begin to emerge out of the quantum world, is only now being revealed.[3] As systems grow in size from the nanoscale to the mesoscale, defects, interfaces, and fluctuations emerge that could be manipulated to program the various desired functionalities of materials, including specific thermal, electronic, and mechanical properties at the bulk level. In this way, nanoscale design can result, at the mesoscale and beyond, in the creation of radically new materials, with properties and functionalities that expand upon, or fundamentally differ from, those found in nature.

Analogous to inorganic materials, living systems demonstrate properties and functionalities that go beyond the additive functions of their constituent parts. The challenge for systems biology is to understand how particular changes to metabolic pathways—often stemming from small changes at the genome scale—play out at the level of the whole organism or an entire microbial community. For example, this latter understanding is critical for achieving effective conversion of biomass into biofuels.[4]

Finally, this new energy research agenda is being shaped by dramatic advances in computation. Today's high-performance computers allow complex real-world phenomena to be studied virtually, including phenomena at the nano- and mesoscale, at very high spatial and temporal fidelity, and at a much-accelerated pace. Critically, these tools are giving access to the properties of systems too dangerous to study experimentally, or too costly to develop by trial-and-error.

Taken together, these developments have put science and technology on the threshold of a transformation from observation to control and design of new systems. This paradigm shift is transforming the processes by which new materials and bio-systems are predicted, designed, and created. This revolution represents a convergence of theory, modeling, synthesis, and characterization, and will enable predictive modeling of materials, control of chemistry, and synthetic biology.[5]

The paradigm of "control" and "design" requires a diverse suite of experimental tools for spatial and temporal characterization and computational tools for theory, modeling, and simulation of complex phenomena. Furthermore, the new energy systems that will usher in a low-carbon, high-efficiency, environmentally sustainable future require a strong disciplinary base and sustained support for new scientific discoveries.

For more than a half century, the DOE Office of Science (DOE-SC) and its predecessor organizations have supported fundamental research underpinning the development and improvement of energy production, conversion, transmission, storage, efficiency, and waste mitigation. This investment is manifested in the broad disciplinary support for scientific discovery at universities and DOE national laboratories,[6] as well as in the development and stewardship of the world's most diverse set of experimental and computational research tools. The federal role in maintaining robust support for scientific discovery is well understood. Perhaps less well known is that the development and construction of these tools, as well as the unique user model that provides open, competitive access regardless of institutional affiliation, is only possible through sustained federal support for these facilities—both in the capital investment to build them and the intellectual investment in the workforce needed to design and operate them. For example, the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory (ORNL) was completed in 2006 after more than five years of construction at a cost of $1.4 billion. Its development and construction was enabled by collaboration of six DOE national laboratories.[7]

This chapter is a survey of how DOE and DOE-SC support energy technology through investment in basic science research and development of complex and unique experimental and computational capabilities. Planning for and development of the capabilities described in this chapter is rooted in both the opportunities presented by basic science and the enabling tools (or lack thereof) needed by the research community to make discoveries. The science and capabilities described in this chapter are also critically important for technology development, enabling discoveries that can obviate the technical roadblocks to broader implementation.

This chapter describes, at a technically approachable level, the unique capabilities that enable both discovery science and technology research and development (R&D), the open-access and merit-based user facility model by which these capabilities are made available to researchers, and the novel DOE funding mechanisms that bring together scientists and technologists around critical issues in energy and the environment to accelerate the transition from scientific discovery to technology deployment. Additionally, a recent scientific study is described for each class of facility. This collection of cutting-edge science is a small subset of DOE-SC-supported basic research that represents how these tools are being used to enable scientific discovery and how these discoveries are connected to the energy technologies reviewed in this report.

9.2 Multidisciplinary, Multiscale Research

The complexity of the scientific problems that must be overcome to realize the energy technologies of the future requires a level of cross-disciplinary insight that is challenging for the single investigator or small research team. In the last decade, DOE has initiated a series of targeted funding opportunities designed to promote this collaborative, multidisciplinary energy science research model. The results of this multi-year effort are the three current research center modalities: 1) the Energy Frontier Research Centers (EFRCs), 2) the Energy Innovation Hubs, and 3) the Bioenergy Research Centers (BRCs). Each has unique structures and modes of operation designed to support their specific research focus.[8] The EFRCs focus on fundamental research,

Five Grand Challenges for Basic Energy Sciences

- How do we control material properties at the level of electrons?
- How do we design and perfect atom- and energy-efficient synthesis of revolutionary new forms of matter with tailored properties?
- How do remarkable properties of matter emerge from complex correlations of the atomic or electronic constituents and how can we control these properties?
- How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things?
- How do we characterize and control matter away—especially very far away—from equilibrium?

addressing one or more of the DOE-SC Office of Basic Energy Science (SC-BES) grand challenges (see textbox: *Five Grand Challenges for Basic Energy Sciences*) and basic research needs (see Section 9.2.1). The Hubs and BRCs are large, comprehensive, multidisciplinary research centers that bridge the gap between basic and applied research to each address a single critical national energy need (see Section 9.2.2). The BRCs are large, multi-institutional, multidisciplinary research centers focused on developing the basic science needed to realize commercially viable cellulosic biofuels (see Section 9.2.3). The overarching goal for all of these research centers is to rapidly enable innovative fundamental energy science research that will form the foundation for the energy technologies of the future, thereby supporting the DOE mission in energy, environment, and national security.

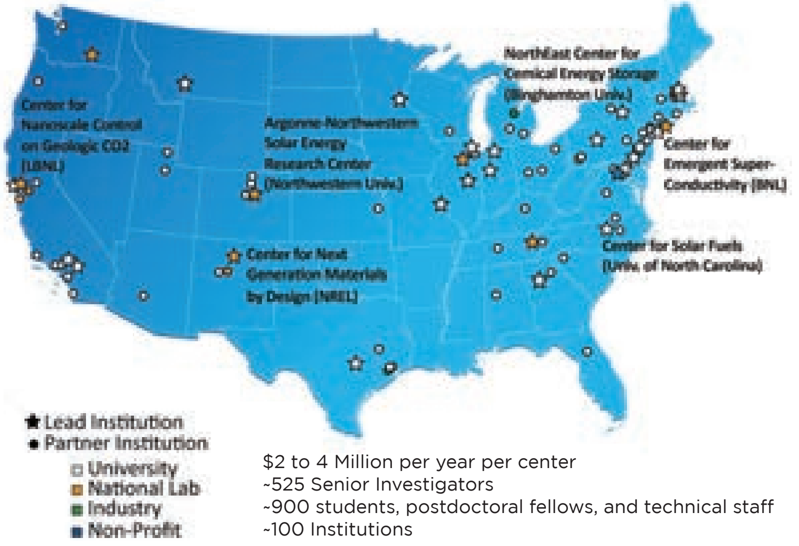
The integrative culture of these research centers is intended to foster the necessary cross-disciplinary collaboration described above, building on a strong disciplinary base built up over the years through sustained investment from DOE, DOE-SC, and other federal agencies.[9] The resulting research partnerships created among universities, DOE national laboratories, nonprofits, and the private sector facilitate knowledge sharing across disciplines so that breakthroughs in one area can quickly be capitalized on and translated to other areas of emphasis, thereby accelerating discovery. This tight integration with DOE national laboratories allows the researchers to leverage the large-scale experimental and computational tools necessary to predict, characterize, and manipulate the behavior of matter at the atomic and molecular scale.

The following sections present more detailed descriptions of the three modalities, including their specific scientific and technical motivations.

9.2.1 Energy Frontier Research Centers

The EFRCs are major collaborative research efforts intended to accelerate high-risk, high-reward fundamental research that will provide a strong scientific basis for transformative energy technologies of the future. Their genesis is in the 2007 Basic Energy Sciences Advisory Committee report, *Directing Matter and Energy: Five Challenges for Science and the Imagination*, the culmination of a series of Basic Research Needs workshops sponsored by SC-BES beginning in 2001.[10] The research at each EFRC must address one or more of five interrelated grand challenges[11] that define the roadblocks to progress and the opportunities for transformational discovery (see textbox: *Five Grand Challenges for Basic Energy Sciences*), as well as one of the priority research directions identified in the BRN workshop series.[12]

Figure 9.1 Locations of Current Energy Frontier Research Centers (EFRC) and Partnering Institutions. The names of a subset of the thirty-two centers are given to show the overlap between EFRC science-drivers and the energy technologies surveyed in this report.



$2 to 4 Million per year per center
~525 Senior Investigators
~900 students, postdoctoral fellows, and technical staff
~100 Institutions

These integrated, multi-investigator centers are tackling some of the toughest scientific challenges hampering advances in energy technologies, including carbon capture and sequestration, predictive modeling of materials, catalysis, and energy storage (see textbox: *Designer Materials for Carbon Capture, Gas Separations, and Catalysis*).[13] The EFRCs are providing an important bridge between basic research and energy technologies through partnerships created between universities, DOE national laboratories, and the private sector, and through the complementarity with other research activities funded by DOE and with the larger energy research community.[14] Figure 9.1 shows the locations of the current thirty-two EFRCs and names six that highlight the overlap between EFRC science-drivers and the energy technologies surveyed in this report.

EFRCs accelerate energy science by providing an environment that encourages high-risk, high-reward research that would be challenging to support at the single investigator level; integrating synthesis, characterization, theory, and computation; developing new, innovative experimental and theoretical tools that illuminate fundamental processes in unprecedented detail; and training an interdisciplinary community of energy-focused scientists.

9.2.2 Energy Innovation Hubs

The four DOE Energy Innovation Hubs[16] focus on overcoming critical scientific barriers that, if realized, could lead to transformative energy technologies. Through the synergistic efforts of large teams of researchers across multiple disciplines and from multiple institutions, including universities, DOE national laboratories, the private sector, and nonprofits, the hubs aim to accelerate the pace of both scientific discovery and technology development and deployment. The ambitious high-risk, high-reward R&D goals within each hub have the potential to provide the breakthroughs needed for revolutionary changes in how energy is produced and used.

The hub model is designed to integrate basic science with applied research and technology development through close links within the hub organization. This organization is inspired by historical research laboratories such as the Lincoln Laboratories at Massachusetts Institute of Technology and the AT&T Bell Laboratories—multidisciplinary research laboratories that conducted groundbreaking science and produced transformative technologies. Furthermore, the hubs have been instilled with a sense of urgency to deliver energy technology solutions and develop deployable new technologies. The hubs are therefore funded at a level to enable this new type of collaboration and strategic coordination between scientists and technologists that is required to fulfill the hubs' broader science and technology missions.[17] Within this model, each hub is unique in how it approaches its goals, which are dictated by the current state of the technology and its associated industry.[18]

Designer Materials for Carbon Capture, Gas Separations, and Catalysis

The ability to efficiently and controllably separate and store different molecules is critically important to a broad range of energy-relevant technologies, including carbon capture, hydrogen storage, chemical sensors, hydrocarbon separations, and chemical production. While possible today, the traditional approaches are energy intensive and therefore costly.

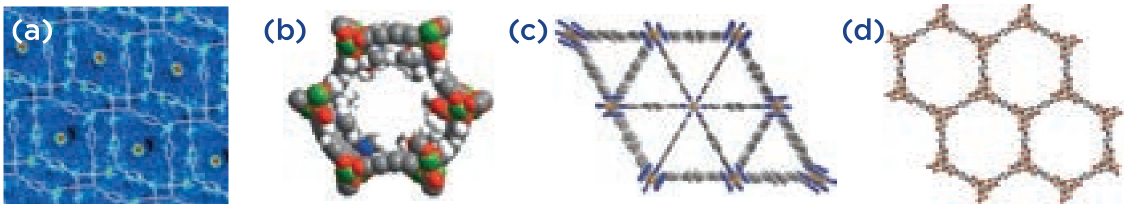
In the last decade, a great deal of scientific and technological attention has been paid to a class of materials known as metal-organic frameworks (MOFs). These highly porous materials typically consist of an array of metallic ion nodes surrounded by organic “linker” molecules, and have extremely large internal surface areas, providing numerous sites for interactions and transport of guest molecules within the MOF pores.

DOE-SC is supporting fundamental scientific research to design, synthesize, functionalize, and characterize MOFs, including work in the core program and the EFRCs. The research to date has resulted in the discovery of new MOFs for the capture of carbon dioxide (CO_2), the separation and storage of hydrogen, the separation of hydrocarbons based on shape, and chemical synthesis such as the conversion of ethane to ethanol (Figure 9.2). Researchers are also working on designing MOFs to withstand the harsh environmental conditions that exist in many potential applications.

Given the very large number of known and possible MOFs, exploring them all experimentally is inefficient. In recent years, significant research has focused on predictive modeling as a means to identify promising candidates for a particular functionality. Those efforts can then guide the targeted synthesis and characterization of a more limited number of materials. The diversity of MOFs is a challenge and an opportunity, both scientifically and technologically. Today’s research holds the promise for a future in which MOFs with tailored multifunctionality are designed on computers and then synthesized for use in a diverse array of energy technologies.

Figure 9.2 The structure of four representative MOFs demonstrates the large diversity within this class of materials. Experiments and computations confirm that these MOFs capture CO_2 (a, b) and separate hydrocarbons (c, d). MOF (d) has also been shown to convert ethane to ethanol.[15]

Credit: (a) From Plonka, A. M., Banerjee, D., Woerner, W. R., Zhang, Z., Nijem, N., Chabal, Y. J., Li, J. and Parise, J. B. Mechanism of Carbon Dioxide Adsorption in a Highly Selective Coordination Network Supported by Direct Structural Evidence. Angewandte Chemie International Edition, 52, 1692–1695 (2013). Reprinted with permission from John Wiley and Sons. (b) Reprinted by permission from Macmillan Publishers Ltd: Nature (519), 2015. (c) From Herm, Zoey R; Wiers, Brian M.; Mason, Jarad A; van Baten, Jasper M; Hudson, Matthew R; Zajdel, Pawel; Brown, Craig M; Masciocchi, Norberto; Krishna, Rajamani; and Long, Jeffrey R. Separation of Hexane Isomers in a Metal-Organic Framework with Triangular Channels. Science, 340, 960-964 (2013). Reprinted with permission from AAAS. (d) Reprinted by permission from Macmillan Publishers Ltd: Nature Chemistry (6), 2014.



The two hubs funded and managed by DOE-SC focus on two challenges in energy: 1) fuels from sunlight and 2) batteries and energy storage. The first hub, the Joint Center for Artificial Photosynthesis (JCAP), aims to demonstrate a scalable, manufacturable solar-fuels generator using Earth-abundant elements that, with no wires, robustly produces fuel from the sun ten times more efficiently than (current) crops (see textbox: *Protected Semiconductors for Solar Fuel Production: A Role for Imperfection*).[19] The primary goal of the second hub, the Joint Center for Energy Storage Research (JCESR), is to enable next-generation batteries ("beyond lithium-ion") for transportation and the electrical grid that scale to five times the energy density at one-fifth the cost relative to a 2011 baseline battery technology.[20]

A third hub, the Consortium for the Advanced Simulation of Light Water Reactors (CASL), managed by the DOE Office of Nuclear Energy (DOE-NE), is developing modeling and simulation tools that will make it possible to predict the behavior of phenomena that define the operational and safety performance of light water reactors (see also Section 9.6.3).[21] These tools have the potential to accelerate the research, development, and demonstration (RD&D) of new nuclear reactor technology. The newest hub, the Critical Materials Institute (CMI), is managed by the DOE Office of Energy Efficiency and Renewable Energy (DOE-EERE). Its mission is to assure supply chains for the rare earth materials critical to clean energy technologies, including strong permanent magnets and lighting phosphors.[22] CMI is fulfilling this mission by developing at least one technology for industry in its first five years in each of three related areas: materials production, waste reduction, and critical materials substitutes.[23]

9.2.3 Bioenergy Research Centers

The BRC Program[25] was established in 2007 by the DOE-SC Biological and Environmental Research (SC-BER) program to accelerate transformational breakthroughs in the basic science needed to develop the cost-effective, sustainable technologies necessary to make cellulosic biofuels commercially viable on a national scale.[26] The three BRCs are multi-institutional, multidisciplinary, and collaborative efforts engaging the universities, DOE national laboratories, the private sector, and nonprofits. They are funded on a large scale[27] to enable research on the entire pathway from bioenergy crop to biofuel production. The three BRCs focus on basic research, pursuing a range of high-risk, high-return approaches to cost effectively produce biofuels and bioproducts from renewable biomass.[28] Additionally, the BRCs track the development of intellectual property to facilitate the transfer of basic science discoveries from the laboratory to the private sector, thereby enabling the translation of their fundamental research advances into the market place.[29]

BRC researchers are taking a multifaceted approach to addressing three grand challenges for cost-effective, sustainable biofuels production. These three grand challenges are encapsulated by the three main facets of the BRC research agenda: 1) create new energy crops, 2) develop new methods for deconstructing lignocellulosic material into chemical building blocks, and 3) insert new metabolic pathways into microbial hosts to increase the production of ethanol and other advanced hydrocarbon fuels that can directly replace petroleum-based fuels such as gasoline on a "drop-in" basis (see textbox: *Improving Biofuel Production through Engineered Inhibitor Tolerance*). Research at the BRCs and in the biofuels community at large is supported and accelerated by continuing development of novel enabling technologies; notably, high-throughput genomic and metabolic screening, synthetic biology, and computational modeling for predicting the effects of genetic manipulation.[30]

9.3 DOE-Supported Research Facilities for Science and Technology RD&D

User facilities are a core component of the DOE-SC mission and an important piece of the broader DOE mission (Table 9.1). Such facilities provide state-of-the-art experimental and/or computational resources to their respective research communities that would be prohibitively expensive to develop, build, and operate by a university, private sector, or nonprofit laboratory. Furthermore, the user facility access model enables the DOE national laboratory complex to bring thousands of outside researchers on-site every year where they can leverage the unique tools and staff expertise for basic science and energy technology RD&D[33] (as well as other areas such as health science and national security) and where they can lend their technical expertise toward the maintenance, development, and application of these tools in support of the broader scientific community.[34]

Protected Semiconductors for Solar Fuel Production: A Role for Imperfection

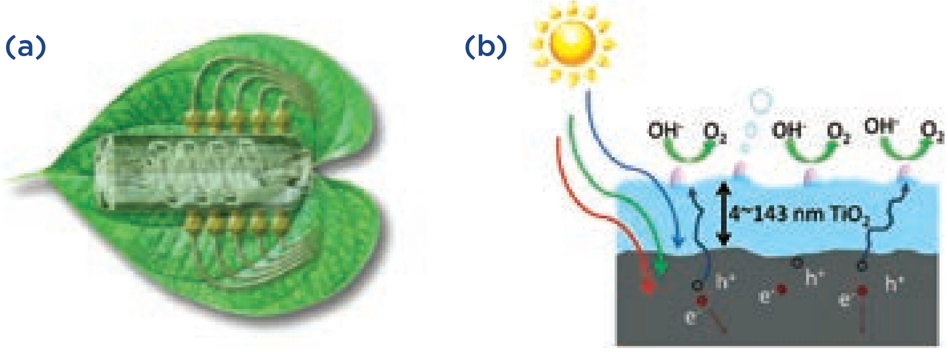
The availability of a solar device that can convert light directly into energy-rich fuels instead of electricity would revolutionize our ability to store energy from sunlight (Figure 9.3a). Given previous investments in developing light-absorbing semiconductors for photovoltaics, it would be advantageous to adapt common photovoltaic materials like silicon and gallium arsenide for use in such a solar fuels generator. Unfortunately, these materials degrade rapidly when submerged in the aqueous solutions that are required to produce fuels.

JCAP scientists have recently discovered a method to protect common semiconductors from corrosion in water while still allowing them to absorb light and generate charge for fuel production (Figure 9.3b). Protective coatings that are sufficiently thick to prevent corrosion typically block incident light or prevent electrical charges produced by the semiconductor from reaching the reactive surface. JCAP researchers used a process called atomic layer deposition to produce a transparent but electrically conductive coating of titanium dioxide on light-absorbing semiconductors. The coating contains imperfections enabling the conduction of charge. By positioning a chemical catalyst on the water-exposed surface of the protective coating, light absorption by the semiconductor and subsequent charge transfer to the catalyst can drive reactions needed for fuel formation.

This strategy of making use of imperfections in the protective coating is an important new tool that could significantly expand the list of candidate materials suitable for use in the solar-driven production of fuels.

Figure 9.3 (a) A solar fuel-generating device would mimic the natural photosynthesis carried out in a leaf, capturing solar energy and converting it into chemical energy stored as a liquid fuel. (b) The titanium dioxide (TiO_2) protective layer stabilizes the silicon photoanode against corrosion so that hydroxide ions (OH-) in the electrolyte can be continuously oxidized to oxygen gas (O_2).[24]

Credit: (b) From Hu, Shu; Shaner, Matthew R.; Beardsless, Joseph A.; Lichterman, Michael; Brunschwig, Bruce S.; and Lewis, Nathan S. Amorphous TiO2 coatings stabilize Si, GaAs, and GaP photoanodes for efficient water oxidation. Science, 344, 1005-1009 (2014). Reprinted with permission from American Association for the Advancement of Science.



Improving Biofuel Production through Engineered Inhibitor Tolerance

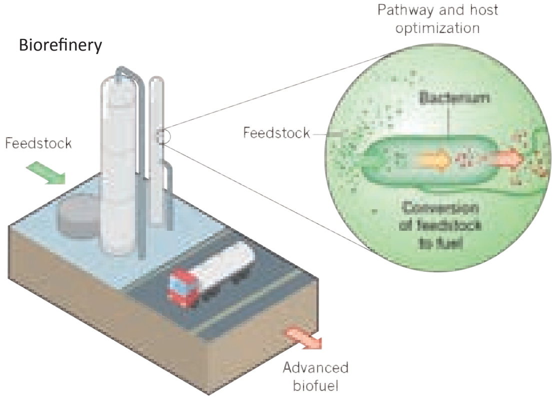
The use of microbial host platforms such as *Escherichia coli (E. coli)* for the production of bulk chemicals and fuels is now a focus of many biotechnology efforts (Figure 9.4). Many of these compounds are inherently toxic to the host microbe, which in turn places a limit on production volume. In order to achieve economically viable production levels, it is necessary to engineer increased output from the production strains while improving tolerance to the desired compounds.

Researchers at the DOE Joint Bioenergy Institute at Lawrence Berkeley National Laboratory (LBNL) discovered an effective method of host engineering for the production of short-chain alcohols. Using systems biology data, the researchers identified forty genes in *E. coli* that show increased activity in response to exogenous isopentenol. This overexpression of several of these candidate genes improved *E. coli* tolerance to the exogenously added isopentenol. Those genes conferring isopentenol tolerance phenotypes belonged to diverse functional groups, including oxidative stress response, general stress response, heat shock-related response, and transport.

To determine if these genes could also improve isopentenol production, researchers co-expressed the tolerance-enhancing genes with an isopentenol production pathway to induce expression. The data show that expression of six of the eight candidate genes improved the production of isopentenol in *E. coli*, with the methionine biosynthesis regulator MetR improving isopentenol production the most. Additionally, expression of MdlB, a transporter protein, facilitated a 12% improvement in isopentenol production. This is believed to be the first example of a transporter being used to improve production of a short-chain alcohol, and provides a valuable new avenue for host engineering in biogasoline production. These results demonstrate that microbial tolerance engineering using transcriptomics[31] data can also identify targets that improve production of biofuels and bioproducts.

Figure 9.4 Optimization of microbial metabolism leads to enhanced production of advanced biofuels such as isopentenol.[32]

Credit: Reprinted by permission from Macmillan Publishers Ltd: *Nature* (488), 2012.



All DOE user facilities are open access,[35] with allocation of time determined by merit-based peer review of user proposals. The submitted proposals are reviewed irrespective of nationality or institutional affiliation, enabling domestic and international scientists from universities, federal laboratories, the private sector, and nonprofits to use the unique capabilities and sophisticated instrumentation. User fees are not charged for nonproprietary research if the user intends to publish the results in peer-reviewed literature; full cost-recovery is required for proprietary research.

User facilities typically are constructed to meet broad mission needs, enabling a range of scientific and technical research, characterization, and analysis.[36] The X-ray light and neutron sources, the nanoscale science research centers, and the Environmental Molecular Science Laboratory, for example, each serve a community of users with representation from across the physical and biological sciences.[37] In contrast, the DOE-SC user facilities such as the Argonne Tandem Linac Accelerator, the Fermilab Accelerator Complex, or the National Spherical Torus Experiment are designed to meet the mission needs of a specific scientific community.

In addition to the twenty-eight DOE-SC user facilities, DOE-EERE, and the DOE-NE support designated user facilities that serve the RD&D needs of specific energy technology communities.

- The Energy Systems Integration Facility at the National Renewable Energy Laboratory (NREL) provides RD&D capabilities for integration of clean energy technologies with the grid. The available capabilities fall into four categories: 1) systems integration, 2) prototype and component development, 3) manufacturing and material diagnostics, and 4) high-performance computing (HPC) and analytics.[38]
- The Nuclear Science User Facilities (NSUF) at Idaho National Laboratory (INL) is the only nuclear energy-designated user facility. It provides users with access to the Advanced Test Reactor, a research-scale nuclear reactor providing large-volume, high-flux neutron irradiation in a prototype environment. NSUF also provides post-irradiation examination facilities as well as beamline capabilities at affiliated partner institutions. [39]

Three user facilities established at ORNL support energy technology RD&D by providing access to state-of-the-art technology and expertise, as well as collaborative access to the DOE-SC experimental and computational user facilities at ORNL (see Table 9.1).

- The Manufacturing Demonstration Facility (MDF) enables rapid development of novel manufacturing techniques that have the potential to produce energy-efficient, competitively priced, high-quality products. MDF capabilities support RD&D in additive manufacturing, composite materials, and carbon fiber, as well as complementary manufacturing research, including lightweight metals processing, roll-to-roll processing, and low-temperature materials synthesis.[40,41]
- The Buildings Technology Research and Integration Center supports technology RD&D to improve efficiency and environmental compatibility throughout the built environment. This broad support for technology development is organized into four Centers of Excellence, three focused on R&D (building envelope, building equipment, and system/building integration), and one on deployment (building technologies deployment). The three Centers of Excellence focused on R&D provide users with unique experimental capabilities to develop and evaluate new technology from concept to commercialization.[42]
- The National Transportation Research Center (NTRC) is supporting industry, academia, and other federal agencies in developing advanced transportation technologies to improve fuel economy, reduce emissions, and address transportation system issues. NTRC provides users with access to a comprehensive suite of experimental laboratories; ORNL supercomputing facilities; and distinctive analysis, diagnostic, and visualization capabilities.[43] NTRC supports the ORNL Sustainable Transportation Program, which is pursuing an “all of the above” transportation research strategy on behalf of DOE.[44]

Finally, the Wireless National User Facility at INL provides researchers with the tools and infrastructure to perform RD&D for infrastructure security, communications interoperability, spectrum utilization, and the reliability of wireless technologies. This work is supported by multiple federal agencies, including DOE.[45]

Table 9.1 Current List of DOE Designated User Facilities[46]

User facility	Location	Description	Program	Section
Wireless National User Facility (WNUF)	Idaho National Laboratory	Wireless communication RD&D	Multiple	9.3
Energy Systems Integration Facility (ESIF)	National Renewable Energy Laboratory	Energy systems RD&D	DOE-EERE	9.3
Nuclear Science User Facilities (NSUF)	Idaho National Laboratory	Nuclear energy R&D	DOE-NE	9.3
Manufacturing Demonstration Facility (MDF)	Oak Ridge National Laboratory	Advanced manufacturing technology RD&D	DOE-EERE	9.3
National Transportation Research Center (NTRC)	Oak Ridge National Laboratory	Vehicle technology R&D	DOE-EERE	9.3
Building Technologies Research Integration Center (BTRIC)	Oak Ridge National Laboratory	Energy-efficient building technology RD&D	DOE-EERE	9.3
Linac Coherent Light Source (LCLS)	SLAC National Accelerator Laboratory	X-ray free electron laser	SC-BES	9.4.1
Stanford Synchrotron Radiation Light Source (SSRL)	SLAC National Accelerator Laboratory	X-ray synchrotron light source	SC-BES	9.4.1
Advanced Light Source (ALS)	Lawrence Berkeley National Laboratory	X-ray synchrotron light source	SC-BES	9.4.1
Advanced Photon Source (APS)	Argonne National Laboratory	X-ray synchrotron light source	SC-BES	9.4.1
National Synchrotron Light Source-II (NSLS-II)	Brookhaven National Laboratory	X-ray synchrotron light source	SC-BES	9.4.1
Spallation Neutron Source (SNS)	Oak Ridge National Laboratory	Pulsed neutron source	SC-BES	9.4.2
High Flux Isotope Reactor (HFIR)	Oak Ridge National Laboratory	Continuous neutron source	SC-BES	9.4.2
Center for Integrated Nanotechnologies (CINT)	Los Alamos and Sandia National Laboratories	Nanoscale science	SC-BES	9.4.3
Center for Nanophase Materials Sciences (CNMS)	Oak Ridge National Laboratory	Nanoscale science	SC-BES	9.4.3
The Molecular Foundry (TMF)	Lawrence Berkeley National Laboratory	Nanoscale science	SC-BES	9.4.3
Center for Nanoscale Materials (CNM)	Argonne National Laboratory	Nanoscale science	SC-BES	9.4.3
Center for Functional Nanomaterials (CFN)	Brookhaven National Laboratory	Nanoscale science	SC-BES	9.4.3
Joint Genome Institute (JGI)	Lawrence Berkeley National Laboratory	High-throughput DNA sequencing and analysis	SC-BER	9.5.1

Table 9.1 Current List of DOE Designated User Facilities (continued)

User facility	Location	Description	Program	Section
Environmental Molecular Sciences Laboratory (EMSL)	Pacific Northwest National Laboratory	Experimental and computational molecular science	SC-BER	9.5.2
Atmospheric Radiation Measurement Climate Research Facility (ARM)	Multiple Sites	Climate observation	SC-BER	9.5.3
National Energy Research Scientific Computing Center (NERSC)	Lawrence Berkeley National Laboratory	High-performance computing	SC-ASCR	9.6.1
Oak Ridge Leadership Computing Facility (OLCF)	Oak Ridge National Laboratory	High-performance computing	SC-ASCR	9.6.1
Argonne Leadership Computing Facility (ALCF)	Argonne National Laboratory	High-performance computing	SC-ASCR	9.6.1
Energy Sciences Network (ESNet)	Lawrence Berkeley National Laboratory	High-performance network for scientific research	SC-ASCR	9.6.2
Facility for Advanced Accelerator Experimental Tests (FACET)	SLAC National Accelerator Laboratory	Linear-accelerator for beam-driven plasma wakefield R&D	SC-HEP	9.7.1
Fermilab Accelerator Complex	Fermi National Accelerator Laboratory	Particle accelerators for HEP research	SC-HEP	9.7.1
Accelerator Test Facility (ATF)	Brookhaven National Laboratory	Laser and electron beams for advanced accelerator R&D	SC-HEP	9.7.1
Continuous Electron Beam Accelerator Facility (CEBAF)	Thomas Jefferson National Accelerator Laboratory	Linear accelerators for QCD research	SC-NP	9.7.1
Relativistic Heavy Ion Collider (RHIC)	Brookhaven National Laboratory	Circular collider for heavy ion research	SC-NP	9.7.1
Argonne Tandem Linac Accelerator System (ATLAS)	Argonne National Laboratory	Superconducting linear accelerator for nuclear structure research	SC-NP	9.7.1
DIII-D Tokamak (DIII-D)	General Atomics	Fusion energy R&D	SC-FES	9.7.4
National Spherical Torus Experiment (NSTX-U)	Princeton Plasma Physics Laboratory	Fusion energy R&D	SC-FES	9.7.4
Alcator C-Mod[47]	Massachusetts Institute of Technology	Fusion energy R&D	SC-FES	9.7.4

The DOE energy technology offices support many unique, specialized facilities at DOE national laboratories (Table 9.2). These shared R&D facilities include a broad spectrum of DOE laboratory assets, such as technology benchmarking test beds (sometimes called "test facilities"),[49] large-scale collaborative R&D centers (see textbox: *Detecting an Elusive Combustion Intermediate*),[50] and specialized materials processing capabilities,[51] among many others.[52] Access to these facilities is made available to external users through collaborative research agreements.[53]

Table 9.2 A Subset of More Than One Hundred Shared R&D Facilities Currently Operating at DOE National Laboratories. Each of the facilities in the table conducts R&D relevant to the energy technologies described in this report.

Shared R&D facility	Laboratory [48]
Materials Preparation Center	The Ames Laboratory
Materials Engineering Research Center	Argonne National Laboratory
Transportation Research and Analysis Computing Center	Argonne National Laboratory
Northeast Solar Energy Research Center	Brookhaven National Laboratory
Magnet Systems	Fermi National Accelerator Laboratory
Biomass Feedstock National User Facility	Idaho National Laboratory
CalCharge Battery Laboratory	Lawrence Berkeley National Laboratory
FLEXLAB	Lawrence Berkeley National Laboratory
Fuels Processing Laboratory	National Energy Technology Laboratory
Solar Energy Research Facility	National Renewable Energy Laboratory
High Temperature Materials Laboratory	Oak Ridge National Laboratory
Applied Process Engineering Laboratory	Pacific Northwest National Laboratory
Combustion Research Facility	Sandia National Laboratories

9.4 Understanding and Controlling Matter: From the Atomic- to the Mesoscale

The twentieth century witnessed revolutionary advances in key areas of basic science underpinning energy technologies, bringing remarkable discoveries such as high-temperature superconductors that conduct electricity with no loss, carbon nanotubes that have a strength-to-weight ratio more than two orders of magnitude greater than steel, and a host of other dramatic developments. Behind these discoveries are extraordinary advances in observation and characterization afforded by today's large X-ray light and neutron sources and a wide range of other sophisticated instrumentation. These tools are providing unprecedented access to the world of atoms and molecules, enabling us to view the atomic-scale structure and dynamics of materials and the molecular-scale basis of chemical processes as never before. This has paved the way for manipulating materials at the nanoscale and the mesoscale to create new tailored functionalities.

The fundamental tenet of materials research is that structure determines function. The practical corollary that converts materials research from an intellectual exercise into a foundation of our modern technology-driven economy is that structure can be manipulated to construct materials with desired properties and behaviors.

Detecting an Elusive Combustion Intermediate

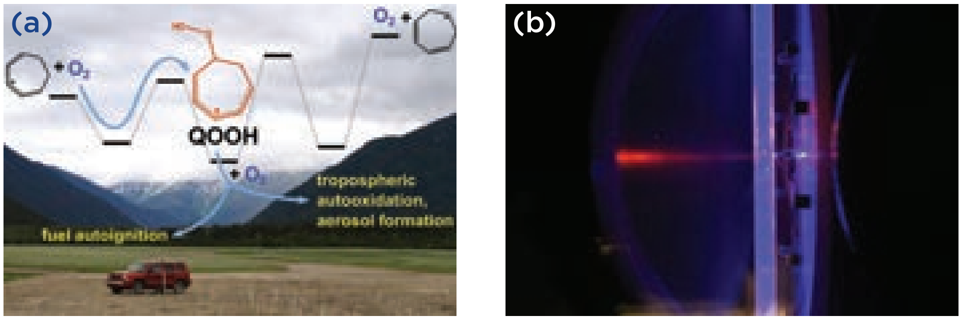
The conversion of organic compounds in Earth's troposphere and the auto-ignition of fuel in internal combustion engines are governed by a surprisingly similar set of reactive intermediates—radicals. Radicals are highly reactive chemical species that have unpaired valence electrons. The presence of radicals leads to the destruction of the ozone layer in the atmosphere and "knocking" in combustion engines.

In combustion engines, a specific class of radicals, called hydroperoxyalkyl radicals and denoted "QOOH," are so short-lived that they are only present in minute quantities and had never been directly detected by experiment. Scientists at Sandia National Laboratories' (SNL) Combustion Research Facility reported in early 2015 direct observation and kinetics measurements of a QOOH intermediate. The path to success was to give the radical a longer life to make its detection easier. The scientists selected a particular species of QOOH radical, where "Q" is a ring of seven carbon atoms (Figure 9.5), that was resonance stabilized (i.e., the electrons were delocalized due to superposition of their wave functions). Simultaneous spectroscopic characterization of QOOH and direct measurement of its reaction kinetics with molecular oxygen was achieved through photoionization mass spectrometry experiments at the Advanced Light Source (ALS) at LBNL. When comparing the reaction of the non-stabilized and resonance stabilized radicals with molecular oxygen, it was determined that the resonance stabilized radical reacts 1,000 times slower.

Decades of previous research had provided evidence that the QOOH radical was a key element in the network of ignition chemistry reactions. The new experimental data from this study can be used to improve the fidelity of models used by engine manufacturers to create cleaner and more efficient cars and trucks.

Figure 9.5 (a) Formation and destruction of the resonance stabilized QOOH (c-$C_7H_9O_2$) radical intermediate. (b) The photoionization mass spectrometry apparatus at the ALS used to detect the short-lived QOOH radical.[54]

Credit: (b) Sandia National Laboratories



As introduced above, a suite of experimental user facilities supported by SC-BES—X-ray light sources, neutron sources, and nanoscale science research centers—are providing researchers with the capabilities necessary to probe the fundamental properties of materials and, subsequently, to manipulate those properties through novel nano- and mesoscale synthesis techniques. The possibilities for the development of novel materials to revolutionize energy technologies are manifold. New generations of electrodes for batteries and fuel cells are being designed to promote the coordinated motion of electrons, ions, and gases and to maximize efficiency and energy density.[55] Mesoporous membranes with defined charge and chemical profiles lining the pores can be designed to separate carbon dioxide, purify water, and catalyze chemical reactions.[56]

The twelve SC-BES user facilities support the basic and applied research activities of thousands of researchers each year from universities, DOE national laboratories, the private sector, and nonprofits. During fiscal year (FY) 2014, the facilities supported more than 15,000 users from many science and technology disciplines, including chemistry, physics, geology, materials science, environmental science, biology, and a wide range of engineering fields. These facilities make possible experimental studies that cannot be conducted in ordinary laboratories, enabling leading-edge research that benefits from a merging of ideas and techniques from different disciplines.

9.4.1 X-ray Light Sources

The laws of physics dictate that it is only possible to “see” objects and structures larger than the wavelength of light used to illuminate them. To probe the atomic and molecular structure of any object, we must use substitutes for visible light, probes that have wavelengths comparable to the distances between the atoms under investigation. X-rays are an essential tool for studying the structure of matter and have long been used to peer into dense material through which visible light cannot penetrate. SC-BES is the premier supporter of X-ray science in the United States and has pioneered the development of virtually all of the instruments and techniques used for research at the light sources.

BES light sources provide open user access to a variety of powerful X-ray probes. The core characteristics of the X-ray light sources make them indispensable tools for the exploration of matter.[57] Synchrotron radiation is characterized by its continuous spectrum, high brilliance, tunability, polarizability, high spatial and temporal coherence, and pulsed incidence. These versatile light sources provide researchers with light at a range of wavelengths capable of probing material structures—at length scales from individual atoms and molecules to biological cells to macroscopic structures. They are important tools for research in materials science, physical and chemical sciences, meteorology, geosciences, environmental sciences, biosciences, medical sciences, and pharmaceutical sciences.

Five X-ray light source scientific user facilities are in operation; four are storage ring-based sources: the ALS at LBNL, the Advanced Photon Source (APS) at Argonne National Laboratory (ANL), the National Synchrotron Light Source-II (NSLS-II) at Brookhaven National Laboratory (BNL), and the Stanford Synchrotron Radiation Lightsource (SSRL) at SLAC National Accelerator Laboratory (SLAC). The fifth facility, the Linac Coherent Light Source (LCLS) at SLAC, is a hard X-ray free electron laser FEL capable of ultrafast, ultra-bright X-ray pulses (see textbox: *Traversing a Catalytic Pathway in Femtosecond Timesteps*). The newly constructed NSLS-II, which started operation in FY 2015, is the world’s brightest storage ring-based light source in the medium-energy range (2–10 kiloelectron Volts [keV]). This tool is giving users unprecedented capabilities for X-ray imaging of energy systems under operating conditions and in real time. In addition to the capabilities described above for LCLS and NSLS-II, the APS, as a hard X-ray source (photon energies above 5–10 keV), emphasizes X-ray scattering. The ALS, specializing in soft X-ray science (photon energies less than approximately 5 keV), emphasizes imaging and spectroscopy in the soft X-ray region. Finally, the SSRL predominantly has beamlines dedicated to X-ray scattering and spectroscopy. Generally, each facility provides core experimental techniques to its user base while emphasizing specific capabilities based on the technical specifications of the facility.[58]

The capabilities of the X-ray light sources have allowed researchers to make incredible scientific discoveries important to both basic and applied energy sciences. The results include real-time structural studies on lithium batteries,[59] imaging of fuel sprays to improve combustion engine efficiency,[60] and mapping the

Traversing a Catalytic Reaction Pathway in Femtosecond Steps

Catalysts are species that alter the pathway of a chemical reaction and lower the energy required to form the desired products. For example, the catalytic conversion of atmospheric nitrogen to ammonia is necessary for fertilizer production that supports agriculture worldwide.

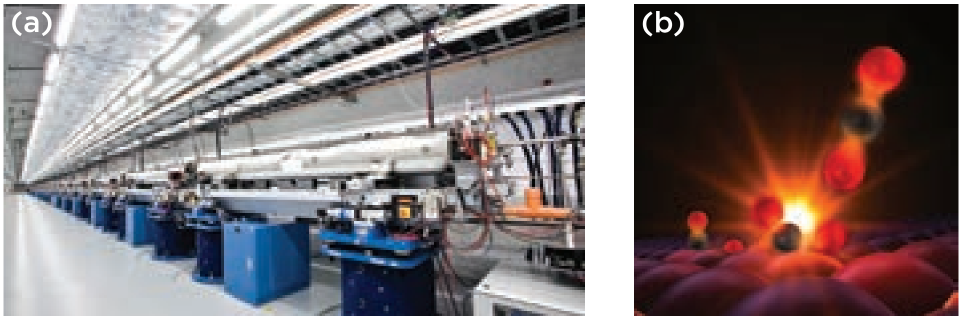
For over a century, scientists have developed theories to predict how chemical species react to form new molecules. Recently, accurate predictions of the rates at which catalytic reactions occur have become accessible, but only for the most elementary reactions and only using idealized catalysts. Experiments have observed chemical bond rupture and formation on catalytic surfaces before and after the event, but not while they occur. By combining theory and experiment, researchers at SLAC National Accelerator Laboratory have now revealed the details of such events by combining ultrafast optical and X-ray laser pulses.

Researchers studied carbon monoxide (CO) oxidation, the same reaction that neutralizes CO from car exhaust. This reaction is also relevant to the conversion of fossil fuels and biofuels into hydrogen gas, a common chemical feedstock and reactant for fuel cells. Following excitation by an optical laser pulse, the ultrafast X-ray pulses available from the LCLS at SLAC—the world's first hard X-ray free electron laser—were used to detect the vibrations of CO and oxygen bound to a ruthenium (Ru) catalyst surface as they reacted to create a new chemical bond and form CO_2. The entire sequence lasts about a picosecond (10^{-12}seconds). Observing the elementary steps of the reaction therefore required making measurements in femtosecond (10^{-15} seconds) steps. Direct measurement of these elementary reaction steps was made possible by combining the ultrafast capabilities of the LCLS with the most advanced theories of chemical bonding and reaction.

In general, the detailed understanding of elementary reaction steps—the holy grail of chemistry—that will be enabled by the LCLS will help realize catalyst development by design. This has the potential to dramatically accelerate the development of new catalysts with specific properties.

Figure 9.6 (a) The 132-meter LCLS undulator hall. (b) Artists concept showing a CO molecule, left, made of a carbon atom (black) and an oxygen atom (red), reacting with an oxygen atom (to the right of CO). The surface of a Ru catalyst holds them in proximity to facilitate their reaction. When excited with an optical laser pulse, the reactants vibrate and the carbon atom forms a transitional bond with the oxygen (center). The resulting CO_2 molecule detaches and moves into the gas phase (upper right).[66]

Credit: SLAC National Accelerator Laboratory



process-structure-property relationships in copper indium gallium selenide, the active material in the Dow Powerhouse™ Solar Shingle.[61] In addition, four of the Nobel Prizes in chemistry from the last decade have been awarded to researchers based, in part, on protein structures determined with data from SC-BES light sources.[62]

The SC-BES light sources will continue to maintain scientific competitiveness and push the boundaries of experimental X-ray science in the years to come.[63] Currently, both the LCLS and APS are in the process of upgrading to extend their capabilities to higher photon energy, brighter beams, and, specific to the APS upgrade, to a far higher degree of beam coherence. These dramatic steps in X-ray beam parameters will allow interfaces, chemical synthesis, and fundamental processes of materials chemistry and physics to be probed under conditions identical to those relevant to energy technologies.[64] Over the next few years, NSLS-II will continue to build out its diverse suite of experimental end stations, opening up its world-leading brightness to a wider range of disciplines and scientific initiatives.[65]

9.4.2 Neutron Sources

Neutron scattering is an outstanding technique for the study of structural and dynamic properties of materials. It finds unique applicability across a spectrum of scientific fields including condensed matter physics, biology, chemistry, polymers, materials science, and engineering.[67] SC-BES currently operates two scientific user facilities for neutron scattering at ORNL: SNS[68] and the High Flux Isotope Reactor (HFIR).[69] The SNS is a pulsed source with nineteen operating beam-lines including eighteen allocated to neutron scattering instruments.[70] It is currently the highest power spallation neutron source in the world. The HFIR provides continuous (non-pulsed) neutron beams to a full suite of scattering instruments that have unique characteristics and are complementary to those at the SNS. The neutrons emitted from either type of source are passed through moderating materials that shift their energy and wavelength into a range useful as a probe of solid and liquid materials. The moderated neutrons are then channeled down flight paths to spectrometers where they interact with a material under study.

The moderated neutrons have wavelengths well matched to the spacing between atoms in materials and thus undergo diffraction from the crystal lattice in a material. This permits the determination of atomic structure in a manner analogous to X-ray diffraction, but with some significant differences. Neutrons are charge neutral and are thus not absorbed by most materials, making them highly penetrating and nondestructive. This provides the opportunity to obtain true three-dimensional structural information from large samples. This property is very important for a number of engineering applications, such as measuring strains in commercial components (see textbox: *New Approaches to Turbine Blade Manufacturing*).[71]

Neutrons possess a magnetic moment and are thereby additionally scattered by any array of magnetic moments within a material, enabling the determination of the magnetic structure simultaneously with the crystal structure. This capability has found unique application to the study of high energy-product permanent magnet materials, colossal magnetoresistive systems, and high-temperature superconductors. Another major unique attribute of neutron scattering as a probe of matter is its sensitivity to light elements. The scattering response of neutrons from both light and heavy elements is essentially equivalent, offering significant advantages for structural studies of soft matter and biological materials that contain mainly light elements such as hydrogen, carbon, nitrogen, and phosphorus. In addition, isotopes of the same element scatter neutrons with different intensity and phase, making possible isotopic substitutions that can enhance or diminish the scattering for specific elements. This unique contrast variation control has proven extremely valuable for the study of many biological systems.

Beyond determining atomic and magnetic structures via diffraction, neutrons can probe longer length scales using reflectometry and small angle neutron scattering (SANS) techniques. Reflectometry provides a depth probe for density or magnetic moment in, for example, polymers and thin films, respectively. SANS has wide

New Approaches to Turbine Blade Manufacturing

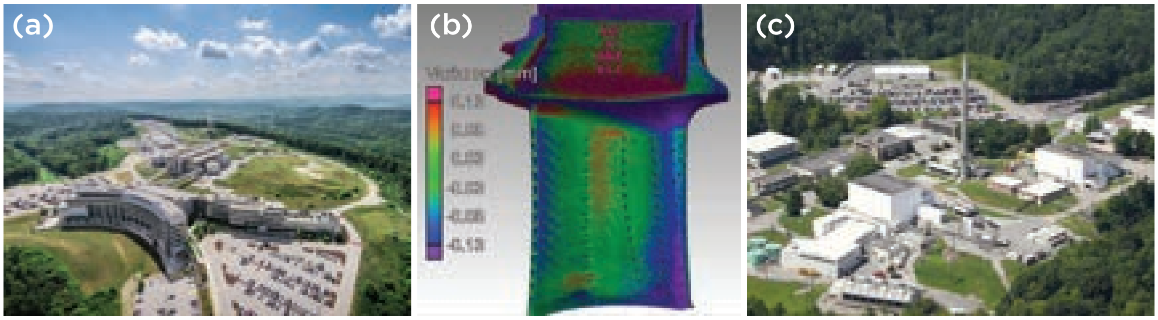
The SNS and HFIR, the SC-BES-supported neutron scattering scientific user facilities at ORNL, provide advanced analytical tools that support development of the next generation of manufacturing technologies (Figures 9.7a and 9.7c). The domestic aerospace industry is leveraging these tools to develop new manufacturing processes and improve on existing ones. These efforts are helping to ensure turbine blades for jet engines produced using these new techniques are of high quality—a characteristic directly related to the safety and fuel-efficiency of the airplane—and to maintain a position of leadership in this global industry.

Neutron computed three-dimensional (3D) tomography is a technique that combines multiple two-dimensional radiographic images to form a 3D image of an object's interior (Figure 9.7b). This technique is enabled by the high penetrating power of the neutron through bulk materials. At the SNS and HFIR, spatial resolutions as small as 75 microns are possible with this technique thanks to novel scintillator detectors developed at ORNL. These detectors convert the neutrons transmitted by the sample into light which is then used to construct the 3D image. Morris Technologies (purchased by General Electric Aviation in 2012) used this tomographic technique on its Inconel 718 turbine blades, which are fabricated using direct laser metal sintering, an additive manufacturing technique.

The neutron tomography results from the SNS and HFIR enabled researchers from Morris Technologies to improve their understanding of the link between residual stress distortions and laser-based additive manufacturing processing of turbine blades with optimized internal cooling structures. This study supports development of highly reliable and reduced cost turbine blades developed using a novel additive manufacturing process.

Figure 9.7 Neutron tomographic imaging techniques available at the DOE-SC neutron scattering scientific user facilities SNS (a) and HFIR (c) were used by Morris Technologies to evaluate internal stresses in turbine blades produced by additive manufacturing (b).

Credit: Oak Ridge National Laboratory



application in studying porous structures and molecular or magnetic clusters in materials. Neutrons also undergo inelastic scattering, in which the energy of the neutron is shifted by interaction with the material.[72] Inelastic scattering has proven to be of great value in understanding many phenomena in magnetism, soft vibrational modes, atomic diffusion, and superconductivity.

Demand for instrument time at both facilities as well as at the National Institute of Standards and Technology Center for Neutron Research[73] far exceeds domestic capacity.[74] In the case of the DOE scientific user facilities, beam time is oversubscribed by a factor of two to five. Furthermore, new research directions in quantum condensed matter, structural biology and biomaterials, soft matter, and energy materials require new capabilities that currently are not available at existing domestic or international facilities. One promising avenue for enabling this new science and increasing available beam time is the proposed Second Target Station at the SNS.[75] This upgrade would provide approximately twenty new state-of-the-art instruments with a focus on techniques that require longer wavelength neutrons and that benefit from a lower neutron pulse rate. It would also increase the intensity of both target stations, thereby reducing the average collection time for an experiment.

9.4.3 Nanoscale Science Research Centers

Nanoscience is the study of materials and their behaviors at the nanometer scale—probing and assembling single atoms, clusters of atoms, and molecular structures. The ultimate goal is to design new nanoscale materials and structures and observe and understand how they function, including how they interact with their environment. Developments at the nanoscale and mesoscale have the potential to make major contributions to delivering scientific discoveries that transform our understanding of energy and matter and advance national, economic, and energy security.[76]

The Nanoscale Science Research Centers (NSRCs) are DOE-SC-sponsored scientific user facilities available for use by the national and international science community to advance scientific and technical knowledge in nanoscale science.[77] The NSRCs are designed to address SC-BES scientific grand challenges (see Section 9.2) in energy and are uniquely structured to address new grand challenges as energy science evolves. The five NSRCs are the Center for Functional Nanomaterials (CFN) at BNL, Center for Integrated Nanotechnologies (CINT) at SNL and Los Alamos National Laboratory (LANL), Center for Nanoscale Materials (CNM) at ANL, Center for Nanophase Materials Sciences (CNMS) at ORNL and The Molecular Foundry (TMF) at LBNL. The NSRCs are housed in purpose-built multi-laboratory buildings and strategically co-located with other DOE scientific user facilities such as X-ray light sources or neutron sources at DOE national laboratories across the United States (see Table 9.1).[78] The in-house and co-located facilities allow the NSRCs to integrate theory, synthesis, fabrication, and characterization in their research activities.

The mission of the NSRCs is to enable the external scientific community to carry out high-impact nanoscience projects and to conduct in-house research to discover, understand, and exploit functional nanomaterials for the benefit of society. To fulfill this mission, the NSRCs house the most advanced facilities for nanoscience research and employ world-class scientists who are experts in nanoscience to help develop these tools and support user research.[79] Each NSRC has distinct, but complementary, scientific themes for its internal staff science program and support a wide range of user activities across the full spectrum of nanoscale science, engineering, and technology with their instrumentation, capabilities, and staff technical expertise. The NSRCs perform primarily basic science and use-inspired basic science. However, applied research and commercialization activities with private sector users are an important part of the NSRC portfolio (see textbox: *"Smarter" Smart Windows Enabled by Nanoscience*).[80]

Although NSRCs perform primarily basic research, they support innovation and applied research with a range of users, including startup companies, large companies, universities, and DOE national laboratories. For example, CFN's polymer nanostructure self-assembly capabilities have helped HGST realize terabit/cm^2 scale magnetic memories for computing and imaging. Chemical synthesis expertise at TMF helped Sematech develop an extreme ultraviolet chemically amplified resist that could be a candidate for microprocessor nodes at less than the current fourteen nanometer scale. CINT's capabilities in nanoparticle synthesis and fluidics led to the launch of Vista Therapeutics' commercial NanoBioSensor™. CNMS expertise in electron microscopy has helped 3M understand performance and durability limitations in fuel cells made with new nanostructured thin film catalysts.

Realizing new materials, creating nanostructures from them, and assembling them into complex structures all require pushing the limits of present synthesis, fabrication, and characterization tools. Understanding the resulting structures requires developing new theories and computational tools that are able to simulate and predict their functionality over a wide range of size and timescales. A major direction of the NSRCs over the next five years is the development of capabilities to create complex nanostructures and observe them under real operating conditions. The NSRCs are planning to develop advanced capabilities in the areas of *in situ*

"Smarter" Smart Windows Enabled by Nanoscience

Nanoscience has led to many discoveries of material properties and new phenomena that have been developed into technologies, including energy technologies, which have generated significant commercial impact worldwide over the past thirty years.[81] At the root of the opportunities provided by nanoscience is the fact that all of the elementary steps of energy conversion (e.g., charge transfer, molecular rearrangement, and chemical reactions) take place on the nanoscale. Thus, the development of new nanoscale materials, as well as the methods to characterize, manipulate, and assemble them, create an entirely new paradigm for developing new and revolutionary energy technologies.

By capitalizing on advances in nanoscale synthesis, researchers from TMF at LBNL have developed a "smart" glass that can switch between blocking visible light, heat-producing near-infrared light, or both, depending on the magnitude of the applied potential. At the heart of the technology is a new "designer" electrochromic material, made from nanocrystals of indium tin oxide embedded in a glassy matrix of niobium oxide (Figure 9.8). Electrochromism is a reversible process that allows the glass to change its transmittance in response to electrochemical charging and discharging. The researchers found a synergistic interaction at the interface between the glassy matrix and nanocrystal, leading to enhancement of the electrochromic effect. As a result, thinner coatings can be used without compromising performance.

This work addresses a critical need for rapid and inexpensive fabrication of stable nanoscale materials that can have tunable electrical and optical characteristics and that can be scaled-up for large area applications. Heliotrope Technologies, an early-stage company, is developing these new materials and manufacturing processes for electrochromic devices with an emphasis on energy-saving smart windows.

Figure 9.8 Nanocrystals of indium tin oxide (blue) embedded in a glassy matrix of niobium oxide (green) form a composite material that can switch between visible or near-infrared light transmitting and blocking states by application of an electric potential. A synergistic interaction in the region where glassy matrix meets nanocrystal increases the potency of the electrochromic effect.[82]

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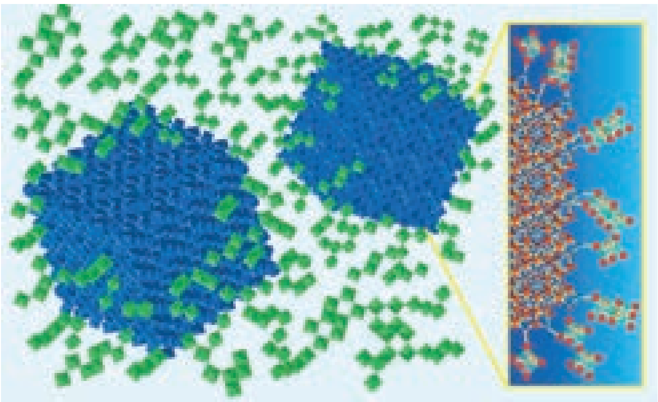


and *in operando* electron microscopy, scanning probe techniques, nanoscience with accelerator-based X-ray and neutron characterization, combinatorial nanomaterials synthesis, and advanced nanofabrication and nanostructure self-assembly (see textbox: *Growing Nano "Hair" for Electrodes*). These new capabilities, coupled with strong user-NSRC staff scientific collaborations, will have a transformative impact on physics, chemistry, materials science, engineering, technology, and many other fields.

9.5 Systems-Based Biological and Environmental Research for Energy

The development of a predictive understanding of energy-relevant biological systems promises new bio-based and bio-inspired technologies for both energy conversion and environmental applications. This understanding is being built on an increasing ability to rapidly decode the genomes of plants and microbes and on a more comprehensive understanding of the complex relationships that mediate the translation of genomics into subcellular and mesoscale macromolecular complexes that shape regulatory and metabolic pathways. The development of new systems approaches and synthetic biology tools are enabling the creation and control of properties and functionalities of biological systems for practical mission outcomes. Because the understanding of biological systems tends to require comparative insights derived from the study of multiple organisms, a key element of this approach is the development and nurturing of a new culture of collaboration among researchers for the sharing of data and resources, with the goal of achieving a community knowledge base to drive further discovery.[84]

New genome-enabled (i.e., "-omics") experimental capabilities and enabling technologies are being developed to achieve improved multimodal measurements of dynamic fluctuations in gene expression, enzyme activity, and metabolite processing at high spatial and temporal resolution. These capabilities leverage the resources of the DOE-SC scientific user facilities, including the X-ray light sources and high-performance computers. These state-of-the-art capabilities enable the scientific community to probe the biological mechanisms that underpin discovery and innovation for future renewable bioproducts and biofuels.

SC-BER seeks to understand the continuum of biological, biogeochemical, and physical processes from the smallest scales (genomes and metabolic pathways) to the largest scales (ecosystems and atmospheric observation). SC-BER strives to describe and explain how genomic information is translated to functional capabilities, enabling more confident redesign of microbes and plants for sustainable biofuels production, improved carbon storage, and understanding of the biological transformation of materials such as nutrients and contaminants in the environment. SC-BER research also advances understanding of how the earth's dynamic, physical, and biogeochemical systems (the atmosphere, land, oceans, sea ice, and subsurface) interact and cause future climate and environmental change, to provide information that will inform plans for future energy and resource needs. All of these efforts are enabled by the three SC-BER supported user facilities described below: the Joint Genome Institute (JGI), the Environmental Molecular Science Laboratory (EMSL), and the Atmospheric Radiation Measurement (ARM) Climate Research Facility. This suite of tools—genomic, analytical, and observational—permit measurements at each scale in the enormous spatial and temporal continuum encompassed by this program, and provide a basis for computationally understanding how the smallest pieces impact the largest systems.

The following three sections describe the facilities that enable the science discoveries described above. This description of the facilities starts at the atomic and molecular scale (e.g., genome sequencing or elemental analysis of aerosol particles) and ends at the global scale (atmospheric observations as input to global climate models). The discoveries described above and in the examples below typically are fundamental in nature, but have an impact—direct or indirect—on the technologies described in this report. At the molecular scale, the tools of the JGI allow researchers to rationally design plants that have significantly higher sugar yields

Growing Nano "Hair" for Electrodes

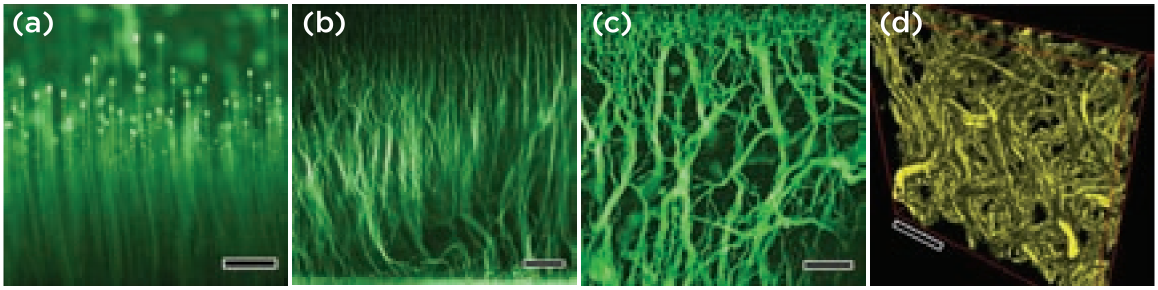
Humankind's ability to create and manipulate the properties of materials has taken much inspiration from the natural world. Biology uses dynamic, out-of-equilibrium processes to assemble cellular components in response to specific signals. Mimicking this assembly approach to organize simple building blocks into complex architectures presents a unique opportunity to learn from nature and go beyond. However, in practice, using this "bottom-up" approach to mesoscale design to form complex structures over multiple length scales has proven to be difficult, since the assembled structures fall apart once the applied stimulus used to direct their formation has been removed.

Inspired by nature, a new self-assembly process has been discovered for fabricating stable 3D structures in response to an applied stimulus. Scientists at ANL using instruments at the CNM developed self-assembled tunable networks of polymer fibers similar to the "hairy" surfaces that exist in our bodies to protect blood capillaries from wear and infection. Using tiny, sticky epoxy droplets as the building blocks, 3D structures ranging from arrays of tiny mushroom pillars (Figure 9.9a) to wavy colloidal "fur" (Figure 9.9b) to highly interconnected networks (Figure 9.9c) were formed on an electrode surface in an electric field. The features of the resulting architectures were tuned by controlling the electric field and droplet surface properties. The structure could then be coated with an atomically thin layer of a conductive material.

This work addresses a critical need for rapid and inexpensive fabrication of stable nano- and mesoscale fibrous materials that can be assembled dynamically and reversibly in response to an applied electric field. Using this approach, tunable 3D architectures can be formed directly on electrode surfaces and further functionalized with conductive materials, which makes this a promising candidate approach for forming low-cost, large surface area electrodes in batteries and organic photovoltaic cells.

Figure 9.9 Control of the synthesis results in a diversity of self-assembled structures formed by sticky epoxy droplets: (a) array of "mushrooms," (b) wavy colloidal "fur," (c) dense fiber network, and (d) a 3D reconstruction of the dense fiber network.[83]

Credit: Reprinted by permission from Macmillan Publishers Ltd: *Nature Communications* (5), 2014 .



needed for biofuel production. At the global scale, the *in situ* observation tools of ARM are yielding better climate models that will produce more accurate forecasts of future energy needs, potentially impacting policy and investment decisions for the technologies described in this report. Each section concludes with a short description of the near-term developmental goals for each facility, and their impact on both science and technology discoveries.

9.5.1 Joint Genome Institute

The mission of the JGI is to advance genomics in support of the DOE missions related to clean energy generation as well as environmental process understanding. JGI provides foundational genomic, bioinformatics, and deoxyribonucleic acid (DNA) synthesis research to underpin cost-efficient production of advanced biofuels and bioproducts from renewable biomass. Operated by LBNL, the JGI is a scientific user facility primarily focused on genome sequencing and interpretation through the Community Science Program, which engages the research community to characterize organisms relevant to DOE science mission areas in bioenergy, global carbon cycling, and biogeochemistry.[85] JGI provides integrated high-throughput DNA and ribonucleic acid (RNA) sequencing and computational analyses that enable systems-based scientific approaches to these challenges.

At its most fundamental purpose, genome sequencing provides the "source code" for biological structures and activities. Even more simply, sequencing generates the "parts list" for an organism or cell. JGI sequencing efforts are providing a large, publicly available database of genetic information that scientists are exploring in search of new capabilities in support of bioenergy research.[86] JGI data contribute to all aspects of the SC-BER Biological Systems Science Program mission space as well as more far reaching explorations of realms of microbiology that will inform future efforts. These include uncovering genomes from previously unexplored regions of microbial taxonomy and elucidating altered "interpretations" (recoding) of DNA sequences in newly sequenced organisms.

A significant part of the JGI mission is to work with the BRCs.[87] Biofuels currently contribute a very small portion of the domestic energy supply.[88] However, the quantity of biomass potentially available for conversion to biofuels exceeds one billion tons annually, which would translate to approximately 30% of current transportation fuel needs.[89] Revolutionary methods for breaking down biomass of a wide diversity of compositions and converting it to fuel compounds or precursors to fuel compounds is a high priority for DOE. The three BRCs (see Section 9.2.3) conduct research on breaking down plant biomass to its cellulose, hemicellulose, and lignin components, and then further reducing these compounds to the component sugar units that are fermented into alcohol-based fuels. JGI's sequencing efforts identify genes whose products may be useful for carrying out these reactions, characterizing variants of genes that may underpin differential properties relevant to biofuel processes, and synthesizing DNA segments useful both as analytic tools and as vectors for new capabilities to enable the BRCs to better carry out their scientific aims.

JGI emphasizes frequent strategic planning in order to keep pace with the extremely dynamic scientific and technological developments in genomics research. The current ten-year vision for the JGI describes its evolution into a next-generation genome science user facility.[90] A primary aim of the JGI is to establish capabilities for functional "annotation" (the assignment of experimentally validated functions) to gene products. Toward that end, massive-scale DNA and RNA sequencing is being supplemented with access to high-throughput experimental and computational capabilities to identify which genes have desired functional properties. Furthermore, large-scale DNA synthesis will be required for both annotation and synthesis of the molecular machinery that will generate tools for deeper analyses as well as, ultimately, the desired products.

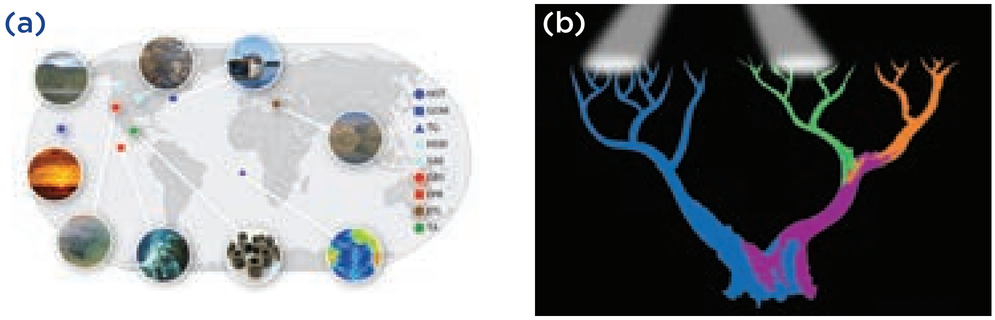
While the quest for sustainable biofuels is a prime mission, it represents only one of several high-level energy and environmental challenges that will be supported by the sequencing capabilities of the JGI. Other examples include improving the growth characteristics of plants through the manipulation of plants, microbes, and their interactions, engineering organisms for improved light capture and energy conversion, discovering and studying new branches of life and new metabolic activities through massive-scale sequencing of unexplored microbial "dark matter" (see textbox: *Illuminating Biology's "Dark Matter": Discoveries from the Deep Space of the Microbial Realm*), and providing the data required to model and predict release of greenhouse gases from warming permafrost.

Illuminating Biology's "Dark Matter": Discoveries from the Deep Space of the Microbial Realm

In cosmology, dark matter is said to account for the majority of mass in the universe; however, its presence is inferred by indirect effects rather than detected through telescopes. The biological equivalent is microbial "dark matter," the unseen majority of microbial life on Earth that can profoundly influence key environmental processes such as plant growth, nutrient cycles, the global carbon cycle, and climate processes. This unexplored realm consists of microbial organisms that cannot yet be directly identified or cultivated in the laboratory and are thus difficult to study and ascribe specific functions through direct observation and manipulation. An international collaboration, led by the JGI, has targeted these uncultivated microbial cells from nine diverse habitats, derived from twenty-eight major previously uncharted branches of the tree of life. Using advanced –omics techniques and computational algorithms, the results fall into three main areas: 1) discovery that metabolic features previously only seen in bacteria are also in Archaea, such as an enzyme used by bacteria to "thin out" their protective cell wall so that the cell can expand during cell division; 2) the ability to correctly assign data from 340 million DNA fragments from other habitats to the proper lineage, linking these fragments to organisms and particular ecosystems, as well as providing insights into possible functional roles; and 3) the ability to more accurately resolve microbial taxonomical relationships within and between microbial phyla, which is critical to predict ecological niches and capabilities. The new results will enable scientists to better predict metabolic properties and other useful traits of different groups of microbes. This work builds upon a JGI pilot project, the Genomic Encyclopedia of Bacteria and Archaea.[91]

Figure 9.10 (a) Samples for metagenomic analyses collected from numerous sites across the globe and sequenced at the JGI have detected numerous previously unknown microbial species. (b) The results shine a metagenomic spotlight on previously unknown areas of the phylogenetic tree, thereby broadening our view of the diversity of the microbial world.[92]

Credit: Joint Genome Institute



9.5.2 Environmental Molecular Science Laboratory

The EMSL, a DOE-SC scientific user facility located at Pacific Northwest National Laboratory (PNNL) in Richland, Washington, leads molecular science discoveries that support the SC-BER and DOE missions that translate to predictive understanding and accelerated solutions for national energy and environmental challenges. EMSL provides premier experimental capabilities, production computing hardware, and software optimized for molecular research to address the fundamental physical, chemical and biological processes that underpin larger-scale climate, energy, and environmental challenges, including novel energy fuels and batteries, and components to enhance energy efficiency in vehicles.[93]

The EMSL solicits research campaigns in its four science themes of atmospheric aerosols, biological dynamics, subsurface and terrestrial ecosystems, and energy materials that combine experimental and computational efforts as well as multiple methods and approaches (see textbox: *Efficiency of Aerosol Particles to Serve as Cloud Condensation Nuclei and Cloud Formation*). Major capabilities provided by the EMSL include magnetic resonance spectroscopy, mass spectrometry, *in situ* imaging, and molecular science computing.[94] These tools are necessary to obtain, for example, a systems-level understanding of how proteomic and metabolomic information are translated into the functional capabilities of living systems, or how the physical and chemical properties at critical interfaces can be tailored for more efficient energy storage and conversion systems. The suite of techniques available at the EMSL are enabling for science across the SC-BER portfolio, including prediction and redesign of metabolic processes,[95] subsurface flow and transport,[96] and modeling and characterization of new energy materials.[97]

The capabilities at EMSL continue to evolve to support characterization of the chemistry and dynamics of molecular species in complex natural systems. The unique 21 tesla high-resolution mass spectrometer[98] will enable EMSL scientists and users to study metabolic processes within and among cells, the composition of organic matter in cells, natural organic matter, secondary organic aerosols, and the formation of aerosol particles. An aberration-corrected dynamic transmission electron microscope will enable users to image dynamic processes within cells/living systems at close to atomic spatial resolution and micro to nanosecond temporal resolution.

9.5.3 Atmospheric Radiation Measurement Climate Research Facility

The largest uncertainty in future climate predictions is how changes in aerosol and cloud properties will interact with the earth's energy balance to either amplify or reduce warming. In order to develop improved predictions of these climate "feedbacks," researchers need extensive observational data to develop more efficient and accurate treatments of aerosol, cloud, and radiative transfer processes in global weather and climate models. The ARM Climate Research Facility is a DOE-SC[100] scientific user facility that develops and manages strategically located *in situ* and remote sensing observatories designed to provide the data necessary to improve the understanding and representation of the radiative impact of clouds and aerosols in climate and Earth system models as well as their interactions and coupling with the earth's surface. This description will help to resolve the uncertainties in climate and Earth system models, supporting development of sustainable solutions for the nation's energy and environmental challenges, including improved confidence in weather and climate predictions that, in turn, enhance public warning capabilities associated with severe weather, and improving tools for energy infrastructure security.

The vision of ARM is to provide a detailed and accurate description of the earth's atmosphere in diverse climate regimes. To that end, ARM capabilities are located across the United States and at select international locations. Three fixed observational sites are located in Oklahoma, Alaska, and the Azores. Three mobile facilities, deployable across the globe,[101] as well as an aerial facility,[102] are designed to address science issues beyond the scope of the fixed observation facilities. All of these facilities are equipped with state-of-the-art remote sensing

Efficiency of Aerosol Particles to Serve as Cloud Condensation Nuclei and Cloud Formation

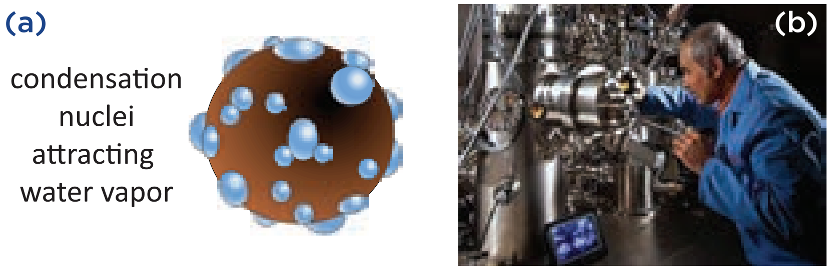
The atmospheric radiative energy balance that, in turn, influences climate variability is strongly influenced by the liquid, ice, and aerosol properties that form cloud condensation nuclei (CCN), the precursors of cloud droplets and cloud formation. Despite numerous field observations of clouds and particles, many uncertainties remain, including the fraction of particles that can become CCN, whether CCN particles are associated with unique chemistry and/or preferred geomorphology, and whether a wider set of particles can lead to different types of CCN. Current cloud microphysics models have taken a simplified approach by identifying only a subset of “qualifying” particles for CCN formation. This results in models that may not represent the full range of atmospheric conditions important to weather and climate, and therefore, high levels of prediction uncertainty in the CCN-affected atmospheric component of the models.

To improve understanding and reduce model uncertainty, a team of researchers involving scientists from the State University of New York at Stony Brook, LBNL, and the College of the Pacific obtained field samples collected in California using ARM. These atmospheric cloud and aerosol samples contained particles with highly variable types of organic compounds coating their surfaces. The ARM data included critical information on the distributions of liquid and ice droplets in each sample as well as the rates of CCN formation within each sample. The physical and chemical properties of the field samples were further analyzed using sophisticated micro-spectroscopy and chemical imaging techniques at the EMSL.

Statistical analysis of the particle properties within and between samples revealed that ice nucleating particles are not dissimilar to droplet nucleating particles. Furthermore, particles that inefficiently produce ice particles can be equally as important as those that efficiently produce cloud droplets, particularly if the less-efficient nucleating particles are abundant in the sample. This study disproved the paradigm that very few types of atmospheric aerosol particles can serve as the seed for ice crystals, showed that a wide variety of particles can lead to ice crystal formation, and revealed that CCN efficiency depends, in part, on organic compounds covering their surfaces. These results are transforming approaches to improve atmospheric and climate prediction models.

Figure 9.11 (a) Under normal conditions, a cloud droplet (and cloud ice particle) requires a microscopic particle on which water vapor can condense. It was assumed that only a small fraction of airborne particles have the right chemistry and/or geometry to condense water vapor. (b) Using samples collected by the DOE ARM facility and chemical imaging and micro-spectroscopic techniques at the EMSL, it was discovered that nearly all classes of particles can serve as cloud condensation nuclei for droplet and ice but with variation in formation efficiency that depends on organic coatings. This new information will be used to improve model parameterizations and reduce uncertainties in climate predictions.[99]

Credit: (a) Center for Multiscale Modeling of Atmospheric Processes; (b) Pacific Northwest National Laboratory



Geoengineering

DOE supports no programs or research and development activities focused on deliberate alterations of the earth's climate, often referred to as "geoengineering." In 2015, the National Academy of Sciences released two reports: *Climate Intervention: Carbon Dioxide Removal and Reliable Sequestration*,[108] and *Climate Intervention: Reflecting Sunlight to Cool Earth*.[109] The first report noted that the costs for removing CO_2 from the atmosphere may be comparable to or exceed those of shifting to lower CO_2-emitting energy sources. The report recommended further research into CO_2 removal strategies in order to, among other goals, identify risks and reduce costs. DOE is supporting RDD&D on CCS, which could be combined with bioenergy systems to provide a net reduction of atmospheric CO_2 (see Chapters 4, 7, and 10). The second report noted the risks of activities known collectively as "albedo modification" were poorly understood. The report recommended against any deployment at "scales sufficient to alter climate," but recommended a research program that focused on multiple-benefit research (e.g., understanding clouds and aerosols), and potentially field experiments at the "smallest practical scales."

instrumentation for measuring atmospheric state variables, trace gases, solar and infrared radiation, surface fluxes, and cloud and aerosol properties.[103] ARM also supports a mobile aerosol observing system that includes capabilities for *in situ* measurements of aerosol chemistry properties.

ARM observations are having a significant impact across the climate research community (see textbox: *Experimental Confirmation of the Greenhouse Effect Due to Carbon Dioxide Emissions*). For example, using ARM observations of the strength of water vapor absorption researchers have substantially improved calculations of far-infrared radiation in radiative transfer models, leading to improvements in a wide variety of atmospheric parameters.[104] Beyond observational efforts, researchers using ARM are developing novel computational models for radiative transfer that increases their efficiency and accuracy in global climate models. Further, the above improvements in radiative transfer modeling and in representations of aerosol and cloud processes in numerical models are having ancillary benefits for solar and wind energy forecasting and for weather forecasting.

Because the accuracy of climate prediction models relies on the quality of parameterizations derived from its data, ARM has steered its priority observations to enhancing our understanding of atmospheric phenomena in regions of high priority scientific interest. The impacts of the warming Arctic basin on cloud physics, changes in aerosol-cloud interactions in the tropics, and the behavior of cloud-aerosol-precipitation interactions during extreme events in all geographic regions are of high priority interest. ARM is adding a very high resolution modeling and simulation component to facilitate and more efficiently link observations to climate model development and predictions.

Climate prediction outputs also serve as input data to integrated assessment and impact, adaptation, and vulnerability models (IAM and IAVM, respectively) that in turn, are built and exercised by the DOE research community. IAMs and IAVMs provide robust evaluations of interdependencies of the energy, water, carbon, and infrastructure sectors, and they can evaluate the sensitivity of model outputs to improved representations of the atmosphere, terrestrial ecologies, and land usage (see also Section 10.4). In particular, the IAMs have the capacity to determine the climate mitigation capacity of emerging low-carbon technologies, such as wind and solar. ARM observations, together with other data from the weather, energy, hydrological sectors, infrastructure, and socioeconomic sectors, will allow next generation models that combine IAMs and IAVMs to evaluate uncertainty and risk associated with a variety of technology development and deployment pathways of relevance to the DOE mission.

Experimental Confirmation of the Greenhouse Effect Due to Carbon Dioxide Emissions

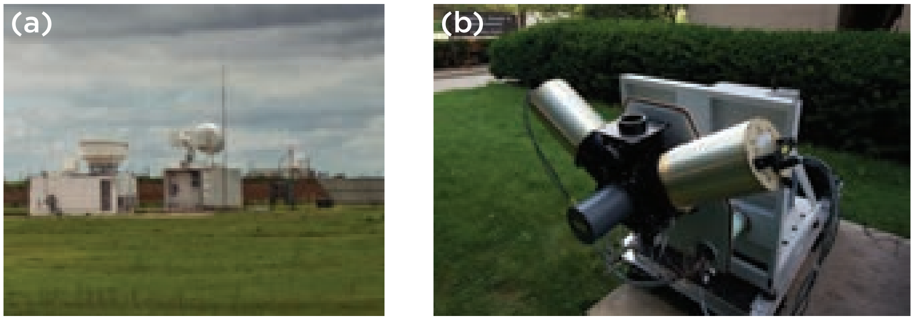
Scientists from LBNL used field observations to confirm directly, for the first time, that increasing levels of CO_2 will warm the atmosphere via the greenhouse effect. The study results are based on observations and other data products collected at the Alaska and Oklahoma ARM sites. Using an eleven-year record of infrared spectral signatures collected at both sites, researchers confirmed previously reported theoretical predictions and laboratory results that indicated increasing atmospheric CO_2 concentrations will lead to increased heating of the atmosphere due to greater absorption of infrared radiation.

Results of the study relied heavily on very precise measurements of the temporal variability of spectral signatures of CO_2, local meteorology, direct measurements of atmospheric CO_2 concentration profiles, removal of the fair-weather bias, and a detailed atmospheric radiative transfer model that included line-by-line spectral radiative transfer and including spectral CO_2 lines. Researchers heavily relied on two instruments designed specifically for ARM facilities. The two atmospheric emitted radiance interferometers (AERIs) were designed to meet the stringent accuracy requirements necessary to carry out this study.

The statistical analysis used to reach the study conclusions used 3,300 daily observations from Alaska and 8,300 daily observations from Oklahoma. Based on data from the AERIs and supporting observations collected at both the Alaska and Oklahoma ARM sites, this study confirmed, for each site, that the theoretical predictions of greenhouse warming were robust and conclusive.

Figure 9.12 Analysis of an eleven-year record of spectral radiance data from ARM sites in Oklahoma and Alaska confirmed theoretical predictions that higher concentrations of atmospheric CO_2 result in increased absorption of infrared energy, and hence atmospheric warming. Until now, the measurement accuracy combined with the length of the data record was inadequate to "prove" beyond doubt that increasing CO_2 must relate to global warming via infrared heating, thus making this analysis groundbreaking. (a) The ARM Oklahoma site. (b) One of the two AERIs that were used to collect the eleven-year data record at both sites.[107]

Credit: ARM Climate Research Facility



ARM observational data are freely available to registered users through the ARM data archive.[105] The value of this data and of the facilities to the climate research community is evidenced by the increase in data downloads from 6.4 terabytes (TB) to 23.7 TB in three years and the corresponding incidence of ARM data citations in the Intergovernmental Panel on Climate Change *Fifth Assessment Report.*[106]

In the next five to ten years, new capabilities for routine large-eddy simulation modeling will be developed to better link ARM observations to the ultimate goal of improving global models. To support this goal, the measurement density around the ARM Oklahoma and Alaska sites will be increased, higher-order data products that are more suitable for model evaluation will be developed, and instrument simulators for more direct evaluation of models with observational data will be developed.

9.6 Modeling, Simulation, and Data Analytics of Complex Phenomena

The scientific developments described in the preceding sections are increasingly being driven by advances in the field of computation, where DOE and DOE-SC are developing and using advanced modeling and simulation techniques to replicate complex real-world phenomena and developing the data analytics capabilities needed to interpret large computational and experimental data sets. The computational capabilities needed to provide these capabilities range from the desktop to the high-performance computer.

Advanced simulation offers the opportunity to move from trial-and-error experimental processes to computational design of materials. New computational capabilities, combined with important theoretical advances, hold the promise for the first time of systematic, theory-based design of new materials *ab initio*, i.e., from first principles. Already, simulations employing a key approach known as Density Functional Theory are being used to identify promising new compounds for a range of applications.[110] The move to design-by-simulation will significantly accelerate the discovery and development of new materials for energy applications.

Computational approaches are not only accelerating the process of genomic sequencing of organisms but also facilitating collaboration and building the comparative knowledgebase that will hold the key to improving our understanding and control over biological systems for energy and environmental applications. In systems biology, with so much diversity, sensitivity to tiny perturbations, and interconnections across a wide range of timescales, advanced computing may well be the only way to fully characterize the dynamics that determine outputs such as biofuel production.

Understanding the earth's climate requires understanding the dynamic, physical, and biogeochemical systems (i.e., the atmosphere, land, oceans, sea ice, and subsurface), and how they interact and cause future climate and environmental change. The inherent complexity of these systems and our limited ability to observe processes and interactions as they occur have proven to be major challenges to predictive climate simulations at the global scale and over extended time frames. Innovative code and algorithm designs are being developed for optimal model computation on current and future high-performance computers. Climate modeling, simulation, and analysis tools will be essential in informing investment decision-making processes for infrastructure associated with future large-scale deployment of energy supply and transmission.

Today's DOE Leadership Computing Facilities have modeled neutron transport in nuclear reactor cores to predict the behavior of nuclear fuels,[111] conducted combustion simulations to increase fuel efficiency,[112] shaped the front ends of long-haul trucks to make them more energy efficient,[113] and simulated ice formation in water droplets to reduce the wind turbine downtime in cold climates.[114] Simulation provides insight into technologies that could not be obtained through testing due to challenges in instrumentation, and saves time and money by reducing expensive and time-consuming testing. The increased physical insight, when coupled with time and money saved, provides U.S. companies with a competitive advantage in moving technologies from the laboratory to production. The next generations of computers will allow even greater understanding and prediction in science and engineering, further accelerating scientific discovery and the creation of complex, engineered systems.

This push to modeling and simulation of real systems is enabled by the parallel development of hardware (computers and networking infrastructure), algorithms, software (operating systems and codes), and personnel. The mission of the Office of Advanced Scientific Computing Research (SC-ASCR) is to discover, develop, and deploy computational and networking capabilities to analyze, model, simulate, and predict complex phenomena important to DOE. The development of these capabilities has been, and continues to be, guided by science needs developed collaboratively with the research community.[110] SC-ASCR's research focuses on the parts of DOE's research agenda that require the most advanced computational capability or novel algorithms.

SC-ASCR has developed multiple approaches to ensure that high-performance computing resources are available, and used, in applied energy areas to advance both basic science and system design. These approaches include ensuring that allocations are available on supercomputers to support research that requires these capabilities,[116] and development of computational tools for DOE science and engineering needs.[117] SC-ASCR has been particularly successful in working with other Office of Science programs through the Scientific Discovery through Advanced Computing (SciDAC) Program. SC-ASCR also works with other programs using approaches such as Hub-based development of new simulation tools,[118] direct integration of simulation with large-scale experimental facilities, and regular communication between DOE-SC and other DOE programs through the Advanced Computing Tech Team (ACTT).[119]

The following sections provide an overview of existing DOE capabilities in computer hardware, networking, and the nonphysical infrastructure required to utilize these resources. Recent examples from research across the DOE computational landscape are provided to demonstrate some of the ways scientific computing is impacting both basic and applied research. Current DOE efforts for increasing computing capabilities by reaching exascale performance levels[120] are discussed, including the potential impact of exascale computing in applied technologies.

9.6.1 Supercomputing Capabilities at the DOE Laboratories

DOE-SC and the entire DOE complex have historically driven development in cutting-edge computing capabilities. Currently, DOE laboratories support four of the top fifteen supercomputers in the world.[121] DOE-SC operates three HPC user facilities: the Argonne Leadership Computing Facility (ALCF), the Oak Ridge Leadership Computing Facility (OLCF), and the National Energy Research Scientific Computing Center (NERSC) at LBNL. ANL and ORNL operate Mira and Titan, respectively, two of the world's fastest supercomputers. These machines are reserved for a small number of projects addressing science and engineering problems that would be prohibitively expensive or impossible to solve on less-powerful machines through allocation processes open to the larger scientific community. The speed of these computers is measured in petaflops (10^{15} floating point operations per second, or pflops).[122] Mira is rated at 8.59 pflops, while Titan is rated at 17.59 pflops with a theoretical peak of more than 27 pflops. This computational power allows these computers to rapidly solve problems that include complex physics over a range of length and timescales. Current science applications include climate simulation, fusion, and atomistic-level simulation of materials.[123]

NERSC operates two pflop machines: Edison (2.6 pflops) and Hopper (1.3 pflops), and is expected to take delivery of Cori (28 pflops) in 2016. NERSC machines are "production" machines; they are used by an extremely wide group of users (5,950 active users from forty-eight states and forty-six countries in FY 2014) for problems that do not require the computing power of the leadership-class machines. NERSC users are drawn from both Office of Science researchers and researchers whose work is aligned with the DOE-SC mission (see textbox: *Nanostructures Half a DNA Strand-Wide Show Promise for Efficient LEDs*).

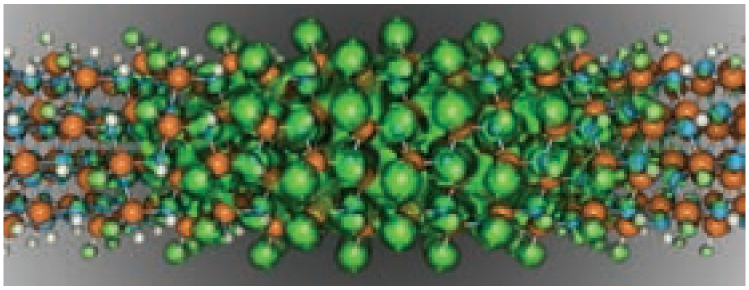
Nanostructures Half a DNA Strand-Wide Show Promise for Efficient LEDs

Light-emitting diodes (LEDs) are semiconductor devices that emit light when an electrical current is applied. At low power, nitride-based LEDs (most commonly used in white lighting) are very efficient, converting most of their energy into light. But efficiency plummets when the power is turned up to levels that could light up a room, meaning a smaller fraction of electricity is being converted to light. This effect is especially pronounced in green LEDs, giving rise to the term "green gap."

Nanomaterials offer the prospect of LEDs that can be "grown" in arrays of nanowires, dots or crystals. The resulting LEDs would not only be thin, flexible, and high-resolution, but very efficient, as well. University of Michigan researchers used supercomputing resources at NERSC to demonstrate that nanostructures half the breadth of a DNA strand could improve the efficiency of LEDs, especially in the green gap region. They found that the semiconductor indium nitride, which typically emits infrared light, will emit green light if reduced in size to a one nanometer-wide wire (Figure 9.13). Moreover, by varying their sizes, these nanostructures could be tailored to emit different colors of light, which could lead to more natural-looking white lighting while avoiding some of the efficiency loss today's LEDs experience at high power.

Figure 9.13 The semiconductor indium nitride, which typically emits infrared light, will emit green light if reduced to a one nanometer-wide wire.[124]

Credit: Lawrence Berkeley National Laboratory



Computing time is allocated by SC-ASCR through a competitive, merit-based proposal review to researchers in the private sector, universities, DOE national laboratories, and other federal agencies.[125] The majority of available time on the leadership-class computers is allocated through two programs: the SC-ASCR Leadership Computing Challenge (ALCC) Program, and the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Program. The ALCC Program provides single-year allocations to research that either contributes directly to DOE's mission, responds to national emergencies, or expands the community of researchers using the leadership class-computing to include new scientific areas. Table 9.3 shows awards made through the 2015 ALCC Program to researchers in energy-related projects.[126]

INCITE awards are multi-year awards targeting computationally intensive, high-impact simulations that require DOE leadership-class computers. The projects represent the most challenging problems, regardless of scientific discipline, and do not necessarily support specific DOE missions. Projects receiving FY 2015 awards included simulations of blood flow during aneurysms, radiotherapy of cancer with ion beams, and

Table 9.3 2015 ALCC Awards Relevant to Energy Technology

Technology area and project title		Institution
Bioenergy	Predictive Modeling of Functional Nanoporous Materials	University of Minnesota
	Developing Hyper-Catalytic Enzymes for Renewable Energy	ORNL
	Molecular Dynamics Studies of Biomass Degradation in Biofuel Production	University of Illinois
Fossil energy	Credible Predictive Simulation Capabilities for Advanced Clean Energy Technology Development through Uncertainty Quantification	ALPEMI Consulting, LLC
	Chombo-Crunch: Modeling Pore Scale Reactive Transport Processes Associated with Carbon Sequestration	LBNL
	Multi-Scale Modeling of Rotating Stall & Geometric Optimization	Dresser-Rand
	Large-Eddy Simulation of Turbine Internal Cooling Passages	General Electric
	System-Level Large-Eddy Simulation of High-Efficiency Gas Turbine Combustors to Advance Low-Emissions Combustion Technology	General Electric
Nuclear energy	Delivering Advanced Modeling & Simulation for Nuclear Energy Applications	ORNL
	Toward a Longer-Life Core: Thermal-Hydraulic CFD Simulations of Deformed Fuel Assemblies	ANL
	Large Eddy Simulation and Direct Numerical Simulation of Fluid Induced Loads on Reactor Vessel Internals	Westinghouse
	High-Fidelity Computations of Fuel Assemblies Subjected to Seismic Loads	George Washington University
Renewable electricity	Computational Design of Interfaces for Photovoltaics	Tulane University
	First Principles Large Scale Simulations of Interfaces for Energy Conversion and Storage	University of Chicago
	Prediction of Morphology and Charge-Transfer Properties in Bulk Material and at Donor/Acceptor Interfaces of Thin-Film Organic Photovoltaic Cells	University of California Los Angeles
	Simulating Multiphase Heat Transfer in a Novel Receiver for Concentrating Solar Power (CSP) Plants	University of Colorado
	Validation of RAP/HRRR for the Wind Forecast Improvement Project II	National Oceanic and Atmospheric Administration
Vehicles	Advancing Internal Combustion Engine Simulations using Sensitivity Analysis	ANL

mapping of southern California's vulnerability to earthquakes. Because many problems in energy are among the most computationally challenging, recent awards have included materials modeling for battery systems, carbon sequestration, simulations of combustion processes, edge plasma transport in tokamak fusion reactors, statewide electric grid optimization (see textbox: *Improving the Energy Grid*), and computational spectroscopy of heterogeneous interfaces for solar energy conversion devices.[127]

Improving the Energy Grid

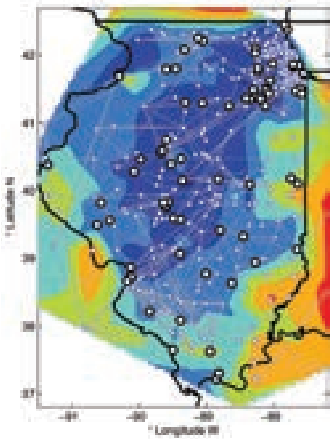
The electrical grid has been described as “the largest and most complex machine ever made.”[128] Accurately simulating this system requires combining the behavior of millions of consumers, the operation of thousands of power plants, weather events, and the decision-making processes of the utilities themselves. Simulating a system with this level of complexity requires high-performance computing. Accurate grid simulation has become even more complex due to changes in the grid, such as the increasing use of weather-dependent solar and wind resources, and sophisticated and highly localized, high-speed decision making at the consumer level. The complexity and range of conditions required for these simulations require stochastic optimization, where the response of the grid to a large sample of random inputs is computed.

High-performance computing can be used to address a key challenge in planning for the future of the electric grid: increasing penetration of wind and solar energy resources. All power plants, conventional or renewable, are subject to outages or changes in power, requiring reserves and other power sources that can be ramped up or down quickly.[129] These changes in output are both more frequent, and less predictable, for weather-dependent renewables such as solar and wind energy. Because reserves are expensive to maintain and operate, finding the minimum required reserves for the expected penetration of these technologies is crucial to affordable deployment.

In 2012, an INCITE-supported team led by ANL used ALCF supercomputing capabilities to demonstrate that up to 20% wind penetration could be accommodated on some configurations without the need for a significant increase in reserves (Figure 9.14).[130] This result showed that new reserves would not be needed to prepare for increased penetration of wind resources, removing another impediment to greater adoption.

Figure 9.14 The features and implied energy prices of the stochastic programming formulation are shown for the state of Illinois. The model contains approximately 2,000 transmission nodes, 2,500 transmission lines, 900 demand nodes, and 300 generation nodes. The needs to be considered over twenty-four successive hourly time periods can reach billions of variables and constraints once the uncertainty in the supply is taken into account.

Credit: Argonne National Laboratory



These results could only be obtained using the newer stochastic methods, and demonstrate the benefits of improved computational tools for grid simulation. SC-ASCR has continued work in this area through the Multifaceted Mathematics for Complex Energy Systems (M2ACS) project, which includes researchers from ANL, PNNL, SNL, the University of Wisconsin, and the University of Chicago.[1311] New grid simulation capabilities can be used to plan for the future of the grid, develop new operational approaches, and predict the impact of grid disruptions due to physical and cyber attacks and natural disasters.[132]

The combination of computational science and domain-area expertise needed to successfully use HPC is often bought to bear on industrially relevant problems through the industrial outreach and partnership programs in supercomputing at ANL, ORNL, and LBNL. The Accelerating Competitiveness through Computational Excellence program at ORNL, the Private Sector Partnership at LBNL/NERSC, and the Industry Engagement Team at ANL, actively work with companies—from start-ups to industry leaders such as Boeing and GE—on problems that require supercomputing. For example, ORNL partnerships with the private sector have developed novel under-the-hood engine designs to reduce drag and improve automotive fuel economy, simulated wind

Optimizing Compression Technology on Titan

To meet the DOE goals of reducing the costs of carbon capture and sequestration (CCS), Dresser-Rand has used Titan through both ORNL's ACCEL Program and SC-ASCR's ALCC Program to optimize novel designs for gas compression systems based on aerospace shock wave compression technology.

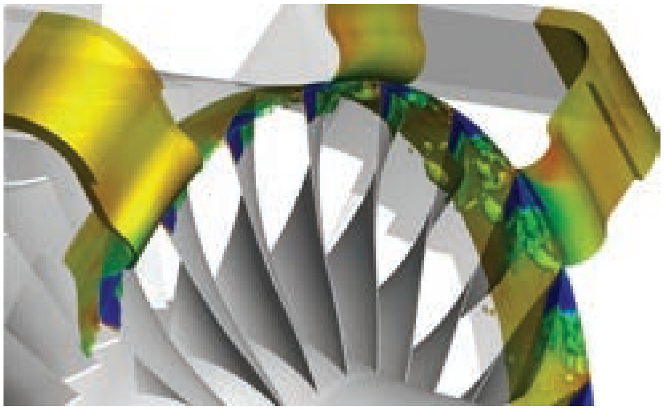
CCS requires energy-intensive pressurization of fossil fuel emissions from power plants to pressures of up to 100 atmospheres. Dresser-Rand estimates its compressor design could reduce capital costs of CCS by 50% and operating costs by 25%. The company's designs are vetted using an ambitious computational method known as intelligently driven optimization, which calculates the best available option within given parameters to predict an optimal design. Using computational fluid dynamics (CFD), the company simulates ensembles containing thousands of designs. A surrogate model approximates the performance of every design perturbation. An evolutionary algorithm is then applied to search the computation space to predict high-performing designs. Once design options are narrowed, the team repeats the optimization process to further refine its search.

To validate its intelligently driven optimization models, the team used Titan to simulate a number of test cases for comparison to a prototype transonic fan stage known as Stage 67, designed and built by the National Aeronautics and Space Administration (NASA) Glenn Research Center. Using the FINE/Turbo CFD code and 1.5 billion grid cells, Titan produced simulation results that not only matched the experimental results, but revealed secondary vortex structures never detected experimentally (Figure 9.15).

These simulations confirmed NASA's experimental finding that a design feature known as tip injection flow control, which recirculates gas flow from downstream of the stage through injectors, can help delay compressor stalls. Ongoing work by Dresser-Rand seeks to use these insights to control stall, which could significantly reduce the energy costs of CCS.

Figure 9.15 Dresser-Rand is simulating equipment that could enable CCS at a significantly lower cost than that offered by conventional equipment. Below is a visualization from a simulation of NASA Glenn Research Center's transonic fan stage experiment prior to stall.[134]

Credit: Dresser-Rand



turbine blade icing in support of new coatings that allow for installation in colder climates, and optimized compression technology that could dramatically reduce the cost of carbon sequestration technology (see textbox: *Optimizing Compression Technology on Titan)*.[133]

HPC within the DOE is not restricted to SC-ASCR facilities. Other DOE laboratories maintain high-performance computers in the pflop range including fifteen of the fastest 150 machines in the world.[130] The National Nuclear Security Administration (NNSA) laboratories have computing needs that require leadership-class computing capability. Lawrence Livermore National Laboratory (LLNL) operates Sequoia (17.17 petaflops) and Vulcan (4.29 petaflops), which have computational capabilities equivalent to Titan and Mira. LLNL makes time on unclassified computing systems, including Vulcan, available to corporate users through the HPC Innovation Center (HPCIC), an alternative to the DOE-SC peer-review-driven models of access. The HPCIC was founded specifically to offer HPC resources and expertise to industrial sponsors whose interests overlap with LLNL's research priorities. The center uses a project-based model where partners pay full cost for projects. LLNL has successfully worked with the California Energy Commission to plan for a future grid with high levels of solar and wind energy resources,[136] and with Navistar, a leading commercial truck manufacturer, to create a more fuel-efficient truck fleet.[137] DOE-EERE's NREL[138] and DOE Office of Fossil Energy's National Energy Technology Laboratory[139] operate their own advanced computing facilities to serve the needs of these programs, and coordinate with SC-ASCR through activities such as the ACTT.

The shared needs of NNSA and SC-ASCR have led to increased collaboration at the technology development and procurement level. Through the Collaboration of Oak Ridge, Argonne, and Livermore (CORAL) Program, SC-ASCR and the NNSA are procuring computers jointly, accelerating technology development while lowering costs. LLNL and ORNL have announced plans to purchase new machines in the 150 petaflop range from IBM. ANL will purchase a different system, as part of a DOE policy to manage technology risk amidst rapid technological change by maintaining architecturally diverse computer systems.[140]

In addition to meeting DOE's advanced computing needs, investments in HPC R&D play a key role in making the resulting technology available to other federal agencies, universities, and the private sector. The National Aeronautics and Space Administration (NASA) and the U.S. Department of Defense have made recent investments in petascale computing hardware. The impact of DOE investment in these areas extends to the private sector as well; approximately thirty of the top 150 HPC systems in the world are in the private sector.

9.6.2 Networking and Data Transfer Capabilities

Modern supercomputing depends on data transfer. The code typically is uploaded by a remote user to be compiled and run on the machine, and the resulting data are returned to the remote user. This must be done with a speed and fidelity that far exceeds the capability of commercial data transmission. The Energy Sciences Network (ESnet) is a dedicated DOE network configured for the data transfer requirements of large-scale science.

While ESnet was originally developed to support computational science needs, its capabilities are increasingly used to transfer large experimental data sets. This is a result of the natural increase in data resulting from the study of complex systems in real time through large-scale experiments. DOE's X-ray light and neutron sources, as well as large international projects like the Large Hadron Collider (LHC), are leveraging ESnet's unique capabilities for real-time analysis of experimental results (see textbox: *Photon Science in the Fast Lane*). This has the effect of both improving resource management at high-demand facilities like the LCLS and facilitating collaboration for international experiments like the LHC.

ESnet was the first continental-scale system in the world to handle data at a rate of 100 gigabits per second (Gbps). While this system takes advantage of commercially-developed hardware, the integration of the system to achieve loss-free transmission of large amounts of data has required unique research and development (R&D). To allow integrated use of experimental and computational tools across DOE facilities, additional

Photon Science in the Fast Lane

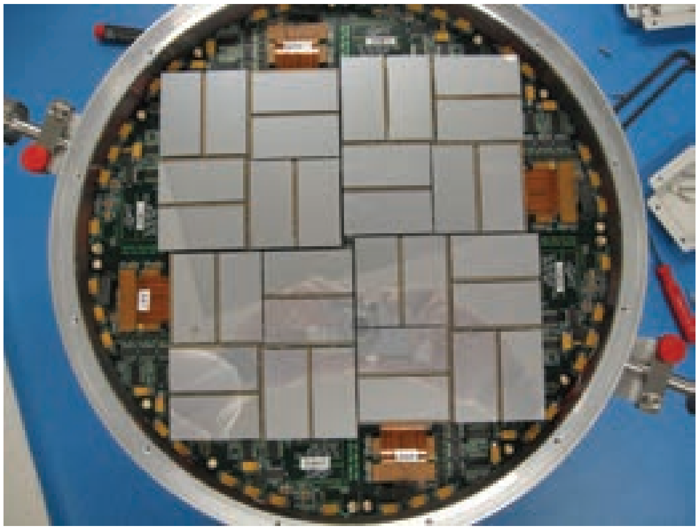
Modern X-ray light sources are instruments uniquely suited to taking pictures at the molecular level. The CSPAD detector (Figure 9.16) at the Coherent X-ray Imaging beamline, one of six beamlines at the LCLS at SLAC, regularly takes 150 terabytes (TB) of data from physical samples to form high-resolution 3D models. These models give scientists an atomic-scale view inside nanoscale phenomena such as photosynthesis and catalysis. However, the computational needs to process these large data sets go far beyond the on-site computational capabilities at SLAC.

In a recent study of photosystem II, a key step in photosynthesis, SLAC researchers used the computational facilities at NERSC to process the raw data into usable models. This, in turn, required rapid and accurate transmission of data. Through ESnet, the light source data was transmitted directly from Cornell-SLAC hybrid Pixel Array Dectector (CSPAD) to NERSC at a sustained rate of 10 Gbps. This allowed the data processing to be scaled up, and enabled rapid distribution of the results to collaborators.

The next generation device, LCLS-II, promises dramatically higher repetition rates as well as increased detector resolution. Taking advantage of the higher resolution imaging made possible by the new instrument will necessarily require higher efficiency processing of the larger data sets. Achieving this goal will require the type of full integration of the instruments with data transmission and analysis using high-performance computers like that pioneered by SLAC, ESNet, and NERSC.

Figure 9.16 The CSPAD camera at the LCLS produces 150 TB molecular "snapshots."

Credit: SLAC National Accelerator Laboratory



provision is made to link closely located facilities, such as the JGI, LBNL, SLAC, NERSC, LLNL, and the SNL California site.[141] ESNet is continually being upgraded to keep pace with the growth in data produced from both modeling and measurement of complex systems, and has been expanded to provide high-speed data transmission from Europe, including direct links to the European Organization for Nuclear Research (CERN).

9.6.3 Nonphysical Infrastructure: Algorithms, Codes, and Personnel

Using supercomputers to simulate complex physical phenomena requires three components in addition to the hardware: 1) numerical algorithms capable of solving the governing equations of the physical phenomena to be simulated; 2) software that implements the algorithm and is written to take advantage of the massively parallel processing; and 3) personnel who understand the physical nature of the simulation problem, the algorithm mathematics, and the challenges of parallelization.

The first step for any simulation is identifying the physical equations that govern the system. Once identified, a physically accurate algorithm to numerically solve these equations can be created. The computational power required to implement the algorithm varies widely based on the nature of the equations being simulated and the level of resolution (in both space and time) needed to accurately incorporate all the physics. In many cases, problems that appear to be fairly different are governed by similar equations and can be solved by similar numerical algorithms. DOE national laboratories have developed general-purpose, numerical tool boxes that are often used as the building blocks of complex simulations for both scientific and commercial engineering applications.[142] CASL, a DOE Energy Innovation Hub (see Section 9.2.2), has developed tools to model the complex physics inside an operating nuclear reactor, a system not amenable to extensive experimental characterization (see textbox: *Westinghouse–CASL Team Simulates High-Fidelity Next-Generation Light Water Reactors*).[143]

Westinghouse–CASL Team Simulates High-Fidelity Next-Generation Light Water Reactors

A team representing Westinghouse Electric Company and CASL performed core physics simulations of the Westinghouse AP1000 pressurized water reactor (PWR) core using CASL's Virtual Environment for Reactor Application (VERA). Westinghouse is deploying the AP1000 worldwide, with eight nuclear power plants currently under construction in China and the United States.

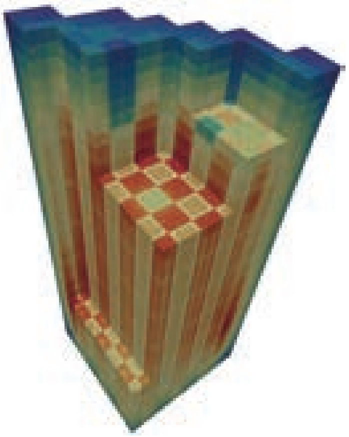
The simulations, performed on Titan at the OLCF, produced 3D, high-fidelity power distributions representing conditions expected to occur during the AP1000 core start-up and used up to 240,000 Titan cores in parallel (Figure 9.17). The results provide insights that improve understanding of core conditions, helping to ensure safe startup of the AP1000 PWR core.

Researchers at CASL have already simulated new reactors under development in South Carolina and Georgia. As computing power increases, CASL will continue to address key nuclear energy industry challenges, including higher fuel burnup and lifetime extension, while also increasing confidence in nuclear safety.

Today, Westinghouse technology is the basis for approximately one-half of the world's operating nuclear plants, including more than 50% of those in Europe. CASL's core partners are a strategic alliance of leaders in nuclear science and engineering from government, the private sector, and universities.

Figure 9.17 Using VERA, CASL investigators successfully performed full core physics power-up simulations of the Westinghouse AP1000 PWR core.[144]

Credit: Consortium for Advanced Simulation of Light Water Reactors



Parallelization of a complex numerical simulation is essential for taking advantage of modern supercomputers and reducing the time required to complete the calculations. Because parallel computing has become the norm for advanced simulation, algorithm development and parallelization can no longer be separate, requiring fundamental understanding of mathematics, computer science and physics that cuts across disciplinary boundaries. DOE's Computational Science Graduate Fellowship was created to ensure that science and technology professionals with advanced computer skills were available for DOE laboratories, as well as for universities and the private sector.[145] Maintaining a core workforce with these skills in DOE national laboratories while also ensuring the same skill sets are available for technology research and development in the private sector and at universities, will enable HPC tools to more broadly impact energy technology development.

Interdisciplinary computational research is also a feature of the SciDAC Program. SciDAC is designed to dramatically accelerate progress in scientific computing to deliver breakthrough scientific results through partnerships of applied mathematicians, computer scientists, and scientists from other disciplines. The current iteration of the SciDAC Program features four institutes: Frameworks, Algorithms, and Scalable Technologies for Mathematics (FASTMath), Quantification of Uncertainty in Extreme Scale Computations (QUEST), Institute for Sustained Performance, Energy and Resilience (SUPER), and Scalable Data Management, Analysis and Visualization (SDAV). These institutes form collaborations with DOE-SC programs to make use of leadership-class computing resources in order to advance scientific frontiers in an area of strategic importance to DOE-SC. These collaborations effectively link scientists with the intellectual resources in applied mathematics and computer science, expertise in algorithms and methods, and scientific software tools at one, or more, SciDAC Institutes. Much of this work translates into energy technology; for instance, the SciDAC partnership with the Office of Fusion Energy Science (SC-FES) has focused on radiation effects in materials, a topic relevant to DOE-NE as well.

9.6.4 Moving toward Exascale Computing

In 2010, SC-ASCR's Advanced Scientific Computing Advisory Committee identified a range of science and technology areas where moving computational power to the exascale (1,000 pflops) had the potential to be truly transformative.[146] These included energy areas such as materials science, combustion, fusion, and fission; related science areas such as climate, biology, and aerodynamics; and nuclear stockpile security. A few of the impacts described in the report are listed:

- **Materials science:** The use of simulation in materials science is limited by the need to capture two length scales: atomistic length scales, which are captured using molecular dynamics, and hydrodynamic effects, which are captured using continuum methods. Bridging these length scales for realistic materials requires simulation of billions of individual atoms over extended timescales, which can only be accomplished using exascale computing.
- **Combustion:** Simulation of combustion is limited by challenges similar to those in materials science: the need to combine multiple physics (e.g., chemical reactions, turbulent fluid mechanics, and heat transfer) into one simulation that bridges length scales from the molecular to the continuum. Exascale simulation enables the most accurate simulation methods to be used for all of the physical phenomena, enabling both new scientific discoveries and design of more efficient combustion systems.
- **Climate:** Exascale computing will enable planet-level climate simulations to move from a grid scale of 100 kilometers (km) to a scale of 3–5 km. This will greatly improve the ability of these simulations to predict the local impacts of climate change.[147]
- **Aerodynamics:** Current aerodynamic simulations for both wind energy and aircraft are limited by one of the classic problems of fluid mechanics: resolving turbulent length scales. Exascale computing will allow simulation of these systems to move from Reynolds-averaged Navier-Stokes models, to large-eddy simulations that capture turbulence with a much greater physical fidelity.[148]

Because of the key role scientific computing plays in DOE's science, energy, and stockpile security missions, SC-ASCR is actively researching both the hardware and software technologies needed to push high-performance computing to the exascale. Key hardware challenges include achieving a massive reduction in power consumption, creating memory systems capable of handling the large amounts of new data produced, and managing the large data flows inside the computer. Major software challenges include creating scalable system software and programming systems, and creating resiliency when individual components in an extreme scale machine fail. Using the new machine architecture will require adapting existing algorithms to work at the exascale and developing new methods for the scientific problems that now become solvable because of exascale computing. Finally, the large amounts of data produced require new approaches to visualizing and processing the data.

One strategy for addressing these challenges is co-design, where the requirements of the scientific problem are considered when first designing the computer system hardware and software. This approach requires coordination among hardware architects, system software developers, domain scientists, and applied mathematicians. Three co-design centers, all targeting problems related to energy—materials in extreme environments, advanced nuclear reactors, and combustion—have already begun preparing simulation methods for this new computational environment.[149] Co-design will ensure that the machines are suitable for DOE applications and allow exascale systems to rapidly be deployed in the development of energy technology.

9.7 Supporting Technologies and Future Energy Sources

Particle accelerators and colliders were developed more than half a century ago to be the workhorse experimental tools supporting development of nuclear fission-based weapons and energy systems and for fundamental discovery in high energy and nuclear physics. Silicon-based detectors were developed soon after to allow researchers to record the aftermath of particle collision events and reveal new fundamental physics.

Today, these technologies form the backbone of the suite of X-ray light and neutron sources and detectors that have enabled the advances in materials science, chemistry, biology, and technology described in this chapter. As they have matured, these technologies have expanded beyond the laboratory, with many applications outside the discovery space, including for medicine, security, environmental stewardship, and manufacturing.

Future experimental tools for scientific discovery and technology research, development, demonstration, and deployment (RDD&D) will undoubtedly be based on cutting edge experimental and computational developments in the modern high energy and nuclear physics communities. This effort is highly interdisciplinary, requiring development of novel materials and synthesis techniques coupled with modeling and simulation. The following four sections review some of the technologies in development for pure scientific research that are poised to become the next generation of experimental tools for energy science and technology.

The first two sections present current developments in accelerator and detector science supported by the Offices of High Energy Physics (SC-HEP), Nuclear Physics (SC-NP), and SC-BES. The motivation for new technology development, the status of selected new technologies, the user facilities that support this work, and the broader applications to technology RDD&D, are discussed.

In the third section, the state of isotope science is presented, focusing on current and future production and on applications to science and technology. Isotopes are critically important for science, energy, manufacturing, health, and national security. Their production is intimately linked to technology development, including accelerators.

The final section looks at development of nuclear fusion as a future energy source. Developing a viable nuclear fusion power device depends on building a foundation of knowledge in plasma science. Development of this foundation is enabled by new experimental and computational tools. This section describes current research into magnetically confined burning plasmas as the basis for a future fusion energy source, discusses the facilities being leveraged to understand and control these plasmas, and describes the interdisciplinary nature of modern fusion research.

9.7.1 Accelerator Science

The next generation of particle accelerators is enabling discovery science across the physical and biological sciences. This is evidenced by the highly collaborative character of accelerator research and development carried out in DOE-SC. Each of the SC-HEP, SC-NP, and SC-BES programs provide support for accelerator R&D specific to their mission needs, including accelerator R&D aimed at improving performance of operating facilities and R&D needs for the development of next-generation facilities within their programs.

SC-HEP is the steward for long-term accelerator R&D and facilitates development of new technologies that enable breakthroughs in accelerator size, cost, beam intensity, and control that are critical to the development of future large-scale particle accelerators[150] and upgrades to existing colliders[151] to reveal new fundamental physics at the energy and intensity frontiers.[152] In SC-NP, accelerators are at the heart of research at all energy levels.[153] Accelerators are also used by the Isotope Program (see Section 9.7.3) to produce radio-isotopes that are in short supply and critical for medicine, science, and national security applications. SC-NP supports development in targetry and accelerator science aimed at improving yields and efficiency of isotope production, as well as capabilities for accelerator-based isotope production. The goals for materials science research in SC-BES—understanding, predicting, and controlling materials properties through characterization of materials composition, structure, and behavior under external perturbation—will see benefits from accelerator developments that increase average photon flux and spatial and temporal coherence in X-ray lasers, as well as higher neutron flux enabled by higher proton currents.

The mission needs articulated in the preceding paragraph can be summarized by the grand challenges for accelerator research—high energy, high power, high gradient, new acceleration methods, beam emittance, brightness and coherence, and compactness.[154] Of critical importance across all three programs is the collaborative development of superconducting radio frequency (SRF) technology and new superconducting magnets.[155] These enabling technologies have the potential to dramatically increase the power, intensity, and efficiency of accelerated beams. SRF technology has already enabled a dramatic increase in the number of particle collisions at the Relativistic Heavy Ion Collider at BNL,[156] and will enable the Continuous Electron Beam Accelerator Facility at the Thomas Jefferson National Accelerator Facility (TJNAF) to double beam energy without new infrastructure development.[157] SRF technology in development at TJNAF and Fermi National Accelerator Laboratory (FNAL) is at the heart of the SC-BES LCLS upgrade (LCLS-II), which will increase brightness and expand the X-ray photon energy range.[158] These developments are enabled by the FNAL Advanced Superconducting Test Accelerator, a fabrication and test facility for superconducting magnets and SRF technology, and the Technology and Engineering Development Facility at TJNAF.[159]

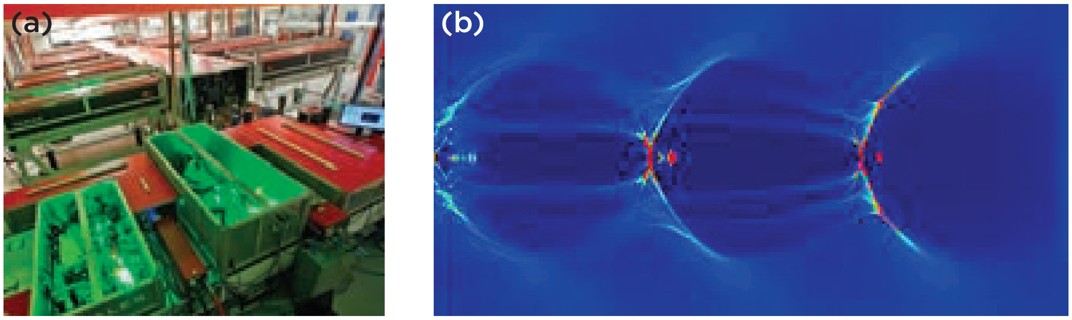
Pushing the frontiers of particle physics requires increasingly higher energies. With current technology, this means larger, more expensive machines. Reducing both the footprint of future accelerators and the cost of fabrication is an important part of the effort to develop plasma wakefield accelerators that can accelerate charged particle bunches to very high energies in a fraction of the distance of traditional, radio frequency-based accelerators.[160] The plasmas are created by very high power lasers or by an accelerated electron (or positron) bunch. The Berkeley Lab Laser Accelerator Center (BELLA), an SC-HEP-supported facility, leverages uniquely powerful optical lasers[161] to produce accelerating gradients up to 100 gigaelectron volts per meter (GeV/m) (see textbox: *Record-Breaking Electron Energies from a Laser-Driven Accelerator*).[162] The need for cutting-edge pulsed lasers leads to a symbiotic relationship in laser technology R&D.[163] The Facility for Advanced Accelerator Experimental Tests at SLAC leverages highly accelerated electrons from the SLAC linac to generate plasma wakefields that accelerate the charged particle bunches at 50 GeV/m, more than 3,000

Record-Breaking Electron Energies from a Laser-Driven Accelerator

Using one of the most powerful lasers in the world, a team of LBNL researchers accelerated subatomic particles to the highest energies ever recorded from a compact accelerator. This setup is known as a laser-plasma accelerator (LPA), an emerging class of particle accelerators that physicists believe can shrink both the cost and size of traditional, miles-long accelerators to machines that can fit on a table. The team used the petawatt laser system at BELLA (Figure 9.18a) to create density waves in a plasma and accelerate electrons in the plasma to 4.2 GeV over a length of only nine centimeters. This energy is the same order of magnitude of electrons operating in today's synchrotron light sources that are hundreds of meters in circumference. Simulations conducted at NERSC (Figure 9.18b) were critical in determining the optimum plasma conditions needed to guide the laser pulse. The results are an important step toward realizing two goals of LPA research: a teraelectron volt-scale electron-positron collider for the high-energy physics community, and laboratory-scale, X-ray free electron lasers.

Figure 9.18 The BELLA laser (a) is a Ti:Sapphire chirped-pulse amplification laser capable of pulsed petawatt level peak power at a frequency of a single hertz. The work was selected as one of ten Best Physics Papers of 2014 by Scientific American. Simulations (b) run at NERSC show a laser plasma wakefield as it evolves in a nine-centimeter long tube of plasma. The charge "wake" (three are shown) allows electrons to "ride" the wake to greater and greater energies.[171]

Credit: Lawrence Berkeley National Laboratory



times the energy gradient of the linac itself. Finally, the Accelerator Test Facility, a scientific user facility at BNL, provides high brightness electron beams and a high-power picosecond CO_2 laser, synchronized to the electron beam, for advanced compact accelerator research.[164] Both of these technologies could form the basis of future X-ray free electron laser user facilities; potentially extend the energy range of existing light sources; and simultaneously provide researchers with pulsed laser irradiation and charged particles for additional studies within the same facility.[165] In addition, plasma-based technologies may enable more compact accelerators for medical or security applications.

Beyond enabling fundamental science broadly across DOE-SC programs, accelerator science has applications in energy technology and the environment. Currently, there are more than 30,000 accelerators in use for medicine, manufacturing, security, and science.[166] In the private sector, applications of accelerated electron beams often center on modification of materials properties. Electron beams are used in the cross-linking of polymers, for surface treatments, and for medical sterilization, among others. Accelerated ion beams are critical to the semiconductor manufacturing industry, enabling doping of silicon-based microelectronic devices, and to the medical device industry, where ion implantation is used to harden materials. Potential new applications of ion acceleration include doping of heterogeneous catalysts and electrodes in energy storage and conversion devices.[167] More generally, replacement of traditional, energy intensive thermal processes with more effective accelerator based technology could realize dramatic energy savings.[168] Greater application of accelerators in the manufacturing, medical, and other industries will require further education of accelerator benefits, as well as cost-effective, compact, and higher-intensity accelerators that can be utilized by individuals or small teams of users.

Electron beam accelerators have been demonstrated as an energy-efficient approach to remediation of waste streams, including flue gas from coal-fired power plants and waste water.[169] In the context of basic science, ion acceleration can simulate the effects on materials of high particle flux from future nuclear fission or fusion devices. Future discovery science accelerators are likely to make increasing use of continuous-wave, high-power, and high-energy beams. Such applications require low loss, high-energy efficiency, high stability, minimal downtime, and lower costs for deployment. The R&D to develop such accelerators in support of DOE-SC's discovery science mission is applicable to the broader DOE energy and environmental missions. The SC-HEP Accelerator R&D Stewardship Program makes modest investments in translational R&D to adapt accelerator technologies for use in energy and environmental applications, among others, and to facilitate private sector collaboration with DOE national laboratories to develop such applications.[170]

9.7.2 Detector Science

X-ray and neutron scattering scientific user facilities operated by SC-BES rely on state-of-the-art detector technology in order to provide experimental data to their large user base. Advances in detector technology are just as critical to the capabilities of these facilities as improvements to the X-ray and neutron sources.

There is a long history of important advances in detector technology first appearing in high-energy physics applications and then being used for other purposes, such as in X-ray scattering at the light source facilities. For example, the particle physics community embraced silicon detectors in the 1970s, and silicon-based hybrid pixel detectors were used at the LHC. This was the first large-scale usage of this detector technology.[172] Today, every major synchrotron light source uses silicon-based detector technology.[173]

In 2012, SC-BES convened a workshop on neutron and X-ray detectors.[174] The resulting workshop report noted that advances in detector technology would be necessary in order to fully take advantage of improvements to X-ray and neutron sources. For example, for an X-ray source of increased brightness, the facility would benefit from more efficient detectors, as well as detectors with faster frame rates and wider dynamic range. These advancements in detector technology will provide new capabilities to the entire user community, such as the capture of motion on very fast timescales of irreversible phenomena.

The workshop report identified several other key parameters for improved detectors, including readout speed, detector efficiency, energy resolution, and dynamic range. In addition, the report noted several priority research directions.[175] One of the highest priorities identified was a replacement for helium-3 (He-3) in neutron detectors (see textbox: *New Developments in Neutron Detection: Addressing the Shortage of He-3*). He-3 is a rare byproduct of tritium decay and has been facing shortages for many years due, in part, to significantly increased usage for national security applications. This has limited the availability of He-3 for the neutron detectors used at neutron scattering facilities. Possible alternatives include lithium-6-doped scintillators and boron-10-doped silicon; however, efficiency improvements will be needed to make these alternatives viable.

9.7.3 Isotope Science

The DOE Isotope Development and Production for Research and Applications subprogram (IDPRA or DOE Isotope Program), managed by the SC-NP, supports the production, distribution, and development of production techniques for radioactive and stable isotopes in short supply and critical to the nation.[176] Isotopes

New Developments in Neutron Detection: Addressing the Shortage of He-3

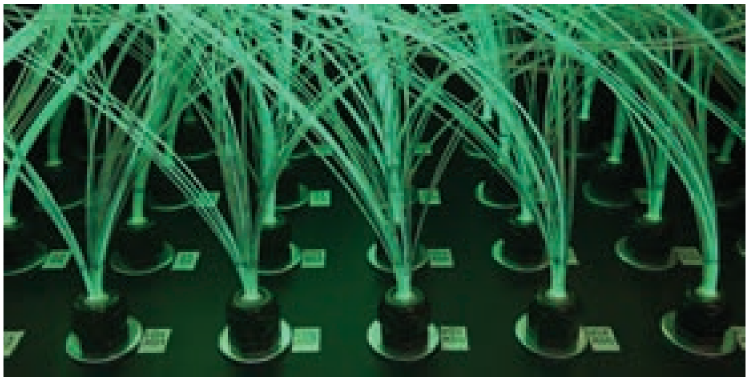
Major advancements in the instrumentation at neutron scattering centers worldwide over the past few years have been accompanied by the increased use of large-scale neutron detectors for enhanced versatility and efficiency of these machines. Additionally, neutron detection for industrial and national security applications is a growing need. Historically, a rare isotope of helium gas, He-3, has been used in these detectors, and the increased demand for neutron detectors has created an extreme shortage of this isotope. This has led to an intense worldwide effort to find alternative types of neutron detectors.

One of the very promising new developments is the wavelength-shifting fiber scintillator detector. This is based on a material that "scintillates," meaning that it emits light when struck by a neutron. The scintillating material emits a blue glow from the impact of a neutron, which is channeled into optical fibers that contain a special dye that converts the blue light created by the scintillator material into longer-wavelength green light (thus the name "wavelength-shifting" fibers) as shown in Figure 9.19. This green light travels through the optical fiber to an array of light detectors called photomultipliers, which convert the green light into electrical pulses that are then easily processed by conventional counting electronics. Proper arrangements of crossed fibers along with electronic decoding hardware further allows the location of the neutrons that strike the scintillator to be determined with an accuracy and counting efficiency that rivals that of current He-3 detectors.

Scientists at the SNS (see Section 9.4.2) have developed arrays of these wavelength-shifting fiber detectors and have deployed them on several neutron scattering instruments with excellent results. Due to the universal applicability of this technology for neutron detection, the SNS has licensed this detector technology to General Electric Reuter Stokes as a commercial product.

Figure 9.19 Optical fibers give off a green glow as they carry light pulses from the scintillator material to an external photomultiplier counting array in the wavelength-shifting optical fiber neutron detector.

Credit: Oak Ridge National Laboratory



are commodities of strategic importance and are essential for energy exploration and innovation, medical applications, national security, manufacturing, and basic research. The subprogram also supports R&D efforts associated with developing new and more cost-effective and efficient production and processing techniques.

The DOE Isotope Program currently supports two accelerator facilities: the Isotope Production Facility at LANL[177] and the Brookhaven Linac Isotope Producer facility at BNL.[178] Reactor-based isotope production is supported at the HFIR (see section 9.4.2) and the Advanced Test Reactor at INL.[179] The Isotope Program also supports the distribution of isotopes with broad importance for energy technology from two NNSA-stewarded facilities: the Savannah River Site Tritium Facilities, (the only domestic supplier of He-3)[180] and the Y-12 National Security Complex (which processes several lithium isotopes).[181] The DOE national laboratory production capacity is augmented by universities performing smaller-scale and unique radioisotope production and R&D.[182] The DOE Isotope Program has made investments at several universities to develop new production capabilities and perform related R&D. The business aspects of the Isotope Program and customer relations are managed by the National Isotope Development Center.[183]

Two of the largest sectors for isotope applications are medicine and national security. In medicine, radionuclides produced by the DOE Isotope Program are used for medical diagnostics and therapeutics, and to support clinical trials of promising new treatments of cancer.[184] The Isotope Program is working to establish large-scale production capability of alpha emitters for cancer therapy, which is a high priority for the medical community, as treatment is limited to only the cancerous tissue in the vicinity of the isotope.[185] In national security, He-3 based neutron detectors are used to monitor cargo entering the United States. Additionally, radioisotopes are used as both calibration standards and sources for nondestructive gamma-ray-based systems for nuclear materials monitoring. Isotopes are also a core component of the current computer-based weapons testing program, providing crucial experimental data to validate computational models.

Both stable and radioisotopes have applications across the physical sciences and engineering sectors. The radioisotopes berkelium-249 and californium-251 are being used to synthesize new super heavy elements and explore the hypothesized "island of stability" in the transuranic elements. In chemistry, biology, and materials science, stable isotopes are a critical tool used to study materials properties (geometric and electronic structure) and (bio) chemical reaction mechanisms. Rare isotopes are at the core of fundamental studies of nuclear physics conducted at the Argonne Tandem Linac Accelerator System at ANL and the future Facility for Rare Isotope Beams at Michigan State University. Silicon-32 is used in oceanographic studies relevant to climate change.

Isotopes are used extensively in the applied R&D, engineering, and manufacturing sectors, often providing irreplaceable capabilities. Besides the use of uranium for reactor fuel, the nuclear power sector utilizes more rare isotopes for selected activities, including californium-252 as a source of neutrons for reactor startup.[186] Isotope-based neutron methods—probes, detectors, and analysis—are employed throughout the energy technology and manufacturing sector. The oil and gas industry uses neutron well-logging, a technique that combines a radioisotope-based neutron source (typically californium-252) with a He-3 neutron detector, to ascertain the hydrocarbon composition of a new well. Gamma radiography using selenium-75, cobalt-60, or iridium-192, allows manufacturers and engineers to assess the integrity of welds for high-pressure vessels and pipelines and determine the extent of corrosion in metals.

The DOE Isotope Program is re-establishing a domestic capability for stable isotope enrichment production and distribution at ORNL (see textbox: *Reestablishing Broad-Scale Stable Isotope Enrichment in the United States*). This is an important asset for the United States, which is currently dependent on foreign sources for many of its stable isotopes.[187] The United States' stable isotope reserve is managed by the DOE Isotope Program, and many

Reestablishing Broad Scale Stable Isotope Enrichment in the United States

From 1945 to 1998, the ORNL calutrons were used to enrich stable isotopes for research and applications. At least 233 naturally occurring isotopes of the first eighty-two elements in the periodic table were enriched during this time. The resulting stable isotope inventory is stewarded by the DOE Isotope Program.

Since 2009, the DOE Isotope Program has supported the development of a modernized research scale electromagnetic isotope separator (EMIS) capability, coupled with small modular centrifuges for stable isotope enrichment at ORNL. The capability is designed to be expandable to produce larger quantities of enriched stable isotopes should the need arise within the federal complex.

Figure 9.20 The EMIS for Stable Isotope Enrichment at ORNL

Credit: Oak Ridge National Laboratory

will no longer be available after depletion of their supply. The development of this capability was recommended by the joint DOE-National Science Foundation Nuclear Science Advisory Committee and will impact a broad variety of applications including medicine, basic research, energy, and national security.

9.7.4 Fusion Energy

Research in SC-FES is developing the scientific basis for a future fusion energy source through support for a hierarchy of topics from basic research to the development of proxies for a self-sustaining burning plasma device.[188] The portfolio includes fundamental research in plasma science, the physics of magnetic confinement of plasmas, two large U.S.-based user facilities, collaboration with major international magnetic confinement devices, strong efforts in theory, modeling, and whole-device simulation, and participation in the construction of the International Thermonuclear Experimental Reactor (ITER) experiment—a facility designed to create a burning plasma operating at a reactor-like scale.[189]

Today, the burning plasma state is approximated with scaled laboratory experiments and computer simulations. The DIII-D National Fusion Facility (DIII-D) is a scientific user facility located at General Atomics and is the largest magnetic fusion research experiment in the United States. It can magnetically confine plasmas at temperatures relevant to burning plasma conditions. Research results from DIII-D will help optimize the tokamak approach to magnetic confinement fusion (see textbox: *Innovative Methods for Controlling Heat Bursts)*.[190] The National Spherical Torus Experiment (NSTX-U) scientific user facility at the Princeton Plasma

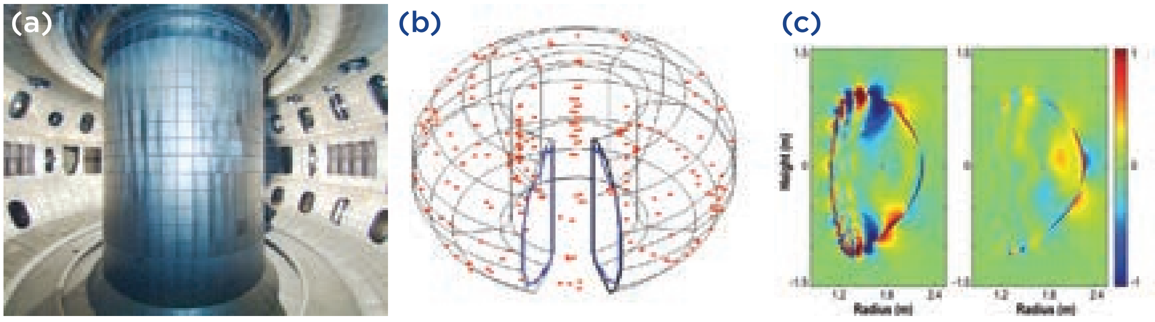
Innovative Methods for Controlling Heat Bursts

Edge localized modes (ELMs) are sudden intense bursts of heat that can erupt from the edge of high-performance fusion plasmas confined in a tokamak with doughnut-shaped magnetic fields. ELMs have the potential for severely damaging the vessel containing the plasma, and have been a major concern for the worldwide fusion research program. Scientists at the DIII-D National Fusion Facility (DIII-D) (Figure 9.21a) have invented a technique for controlling ELMs by applying small, localized 3D magnetic perturbations. This novel technique has revolutionized the science of mode control, and the U.S. fusion program is now designing similar control coils for the International Thermonuclear Experimental Reactor (ITER) fusion facility under construction in Europe.

Quite recently, U.S. scientists have made a major breakthrough in gaining a detailed understanding of exactly how these magnetic perturbations control the ELM bursts. A multi-institutional team of researchers—including scientists from General Atomics, Princeton Plasma Physics Laboratory, ORNL, Columbia University, Australian National University, the University of California-San Diego, the University of Wisconsin-Madison, and several other groups—discovered that the 3D perturbations produce a ripple in the magnetic field near the plasma edge, allowing more heat to leak out smoothly at just the right rate to avert the intense heat bursts. Researchers applied the magnetic fields by running electrical current through coils around the plasma. A new system of approximately one hundred pickup sensors (Figure 9.21b) then detected the plasma response, much as the microphone on an electric guitar picks up string vibrations. These results suggest that this technique can be optimized for eliminating ELMs in ITER and future fusion devices (Figure 9.21c), thus providing a solution to overcoming a persistent barrier to sustained fusion reactions.

Figure 9.21 (a) Inside the DIII-D Tokamak. (b) The position of approximately one hundred magnetic sensors (red dots) recently installed around the plasma. (c) Simulations of the cross-section of the DIII-D plasma show the response typical of non-suppression (c, left) and ELM suppression (c, right), in agreement with experimental measurements.[194]

Credit: (a), (b) DIII-D/General Atomics (c) Reprinted with permission from Paz-Soldan, C.; Nazikian, R.; Haskey, S.R.; Logan, N.C.; Strait, E.J.; Ferraro, N.M.; Hanson, J.M.; King, J.D.; Lanctot, M.J.; Moyer, R.A.; Okabayashi, M.; Park, J-K.; Shafer, M.W.; Tobias, B.J. "Observation of a Multimode Plasma Response and its Relationship to Density Pumpout and Edge-Localized Suppression," *Physical Review Letters* (114:10), p. 105001-1-5. Copyright 2015 by the American Physical Society.



Physics Laboratory has a more compact spherical torus configuration that could lead to the development of smaller fusion devices. With the recent upgrade, the NSTX-U facility is the world's highest-performance spherical torus device. These two plasma science user facilities are complementary, with their unique geometries allowing both to serve as world-leading scientific platforms for fundamental burning plasma science.[191]

Development of sustained burning plasma fusion devices requires a collaborative research effort across the experimental and computational arenas. The materials used in a magnetic confinement device must withstand enormous heat and neutron fluxes, and fluxes can qualitatively change materials strength and characteristics due to atom displacement. The development of new materials that can tolerate the extreme conditions of a burning plasma environment requires leveraging the tools of synthesis, fabrication, characterization, and computation described earlier in this chapter. The SC-FES program is an active participant in SC-ASCR's multi-institutional and interdisciplinary SciDAC Program, leveraging the leadership-class computing resources of DOE-SC to address challenges across the fusion science space, including magnetic confinement and computational fusion materials science.[192] These simulations provide the basis for comparison to detailed measurements and increasingly represent tools for discovery.

The fusion enterprise supports, and is in turn supported by, broader research in plasma science that targets the understanding of an enormous range of phenomena, from those occurring at the galactic scale to plasma science applicable to the world of microelectronic and nanoscale fabrication.[193] Plasma science supported by SC-FES is central to many science and technology issues, from formation of galactic jets and accretion of stellar material around black holes to optimization of processes in the semiconductor industry and development of technologies deployed for national defense, medical applications, and homeland security. This research is carried out by universities, private R&D groups, and DOE national laboratories.

9.8 Conclusion

This chapter describes the suite of scientific user facilities and multidisciplinary research centers for the nation that are currently supported by DOE. The chapter also provides a small sample of the scientific research that these facilities enable. These examples illustrate the potential of fundamental scientific research to impact the energy technologies described throughout this report.

The analysis of R&D needs presented in the preceding chapters of this report reveal two crosscutting scientific themes: 1) new materials; and 2) modeling, simulation, and analytics. Through careful strategic planning, DOE-SC is well-positioned to continue to support key scientific research that will lead to the necessary advances in these areas. Efforts led by the SC-BES program to explore the opportunities in materials science have led, for example, to the report *Computational Materials Science and Chemistry*,[195] which looked at how simulation can be used to accelerate material discovery and understanding, and *From Quanta to the Continuum: Opportunities in Mesoscale Science*,[196] which looked at how emergent mesoscale phenomenon can be harnessed for science and energy.

Future developments in both computational materials science and in SC-BES scientific user facilities, specifically the LCLS–II and the APS upgrade, are important to the materials science community. Sustained investment in these areas can benefit a wide variety of scientific disciplines, and can address many of the energy-related materials science needs described in the preceding chapters.

Similarly, advanced modeling, simulation, and large-scale data analytics are a priority for meeting national science and energy needs. The investments in new, more powerful computers, through the CORAL collaboration, at ORNL, ANL, and LLNL, and in exascale computing, are vital for science and technology development moving forward. It is critical to develop and disseminate new computational tools across its mission areas. Enabling the effective use of high-end computation across the entire science, energy, and nuclear security portfolio—one of the core missions of the ACTT—will facilitate addressing many of the energy-related problems discussed in this report.

Supplemental Information

A Comparison of Research Center Funding Modalities

High-Performance Computing Capabilities and Allocations

User Facility Statistics

Examples and Case Studies

[See online version.]

Endnotes

[1] More information about the National Nanotechnology Initiative can be found at http://www.nano.gov.

[2] "Nanoscience Research for Energy Needs." Report of the National Nanotechnology Initiative Grand Challenge Workshop, March 16-18, 2004. Available at: http://science.energy.gov/~/media/bes/pdf/reports/files/nren_rpt.pdf.

[3] "From Quanta to the Continuum: Opportunities for Mesoscale Science." Report for the Basic Energy Sciences Advisory Committee Mesoscale Science Subcommittee, September 2012. Available at: http://science.energy.gov/~/media/bes/pdf/reports/files/OFMS_rpt.pdf.

[4] Bioenergy Research Centers, U.S. DOE, Office of Science, Office of Biological and Environmental Research, February 2014. See http://genomicscience.energy.gov/centers/BRCs2014HR.pdf.

[5] For more on predictive theory and modeling of materials, see "Computational Materials Science and Chemistry: Accelerating Discovery and Innovation Through Simulation-Based Engineering and Science." Report of the Department of Energy Workshop on Computational Materials Science and Chemistry for Innovation, July 26-27, 2010. Available at: http://science.energy.gov/~/media/bes/pdf/reports/files/cmsc_rpt.pdf.

[6] The DOE-SC supports basic research across six programs—Basic Energy Sciences, Biological and Environmental Research, Advanced Scientific Computing Research, High Energy Physics, Nuclear Physics, and Fusion Energy Sciences. Each of these programs is subdivided into multiple core scientific disciplines. Descriptions of the core research programs are available at http://science.energy.gov/programs/.

[7] SNS (see Section 9.4.2) was developed through collaboration of ANL, BNL, LBNL, LANL, ORNL, and TJNAL. When completed in 2006, it became the world's most powerful pulsed neutron source.

[8] A table comparing the three types of multi-institutional research centers across institutional participation, award length and management, funding level, and research focus is provided in Supplemental Information (section 9A).

[9] An interactive map of DOE-SC grant award data and cooperative agreements for FY 2014 is available at http://science.energy.gov/universities/interactive-grants-map/. This information can be parsed in multiple ways, including by DOE-SC program, by institution (e.g., educational institution, for-profit organization, small business, or other federal agency), or by program area/topic (e.g., catalysis science, physical behavior of materials, or solar photochemistry).

[10] Examples of Basic Research Needs (BRN) workshops are Basic Research Needs for the Hydrogen Economy, Basic Research Needs for Solar Energy Utilization, Basic Research Needs for Solid-State Lighting, and Basic Research Needs for Advanced Nuclear Energy Systems. A hyperlinked list of all the BRN reports is found in Supplemental Information (Chapter 1).

[11] The five SC-BES grand challenges are presented in "Directing Matter and Energy" available at: http://science.energy.gov/~/media/bes/pdf/reports/files/gc_rpt.pdf. The grand challenges addressed by current and former EFRCs are provided at http://science.energy.gov/bes/efrc/research/grand-challenges/ and http://www.science.energy.gov/bes/efrc/history/grand-challenges.

[12] Each BRN workshop identified a set of priority research directions for the respective scientific community.

[13] The full list of EFRCs, partnering institutions, and research descriptions is available at http://www.science.energy.gov/bes/efrc/centers. Technical summaries for each EFRC are available at http://science.energy.gov/~/media/bes/efrc/pdf/technical-summaries/ALL_EFRC_technical_summaries.pdf.

[14] The EFRCs have established a community Web site at http://www.energyfrontier.us/ to share research and facilitate communication between the EFRCs, researchers, and SC-BES.

[15] (a) Plonka, A. M.; Banerjee, D.; Woerner, W. R.; Zhang, Z.; Nijem, N.; Chabal, Y. J.; Li, J.; Parise, J. B. “Mechanism of Carbon Dioxide Adsorption in a Highly Selective Coordination Network Supported by Direct Structural Evidence.” *Angewandte Chemie* International Edition (52:6), 2013; pp 1692–1695. Available at: http://onlinelibrary.wiley.com/doi/10.1002/anie.201207808/abstract; (b) McDonald, T. M.; Mason, J. A.; Kong, X.; Bloch, E. D.; Gygi, D.; Dani, A.; Crocellà, V.; Giordanino, F.; Odoh, S. O.; Drisdell, W. S.; Vlaisavljevich, B.; Dzubak, A. L.; Poloni, R.; Schnell, S. K.; Planas, N.; Lee, K.; Pascal, T.; Wan, L. F.; Prendergast, D.; Neaton, J. B.; Smit, B.; Kortright, J. B.; Gagliardi, L.; Bordiga, S.; Reimer, J. A.; Long, J. R. “Cooperative Insertion of CO2 in Diamine-appended Metal-organic Frameworks.” *Nature* (519), 2015; pp 303-308. Available at: http://www.nature.com/nature/journal/v519/n7543/full/nature14327.html; (c) Herm, Z. R.; Wiers, B. M.; Mason, J. A.; van Baten, J. M.; Hudson, M. R.; Zajdel, P.; Brown, C. M.; Masciocchi, N.; Krishna, R.; Long, J. R. “Separation of Hexane Isomers in a Metal-Organic Framework with Triangular Channels.” *Science* (340), 2013; pp 960-964. Available at: http://www.sciencemag.org/content/340/6135/960.full?sid=14f2af9d-dc94-4005-8ba7-58a97fe59d54; (d) Bloch, E. D.; Queen, W. L.; Krishna, R.; Zadrozny, J. M.; Brown, C. M.; Long, J. R. “Hydrocarbon Separations in a Metal-Organic Framework with Open Iron(II) Coordination Sites.” *Science* (335), 2012; pp 1606-1610. Available at: http://www.sciencemag.org/content/335/6076/1606.full?sid=cb7c8938-40a3-453d-b45b-258787d9a0a8. (e) Xiao, D. J.; Bloch, E. D.; Mason, J. A.; Queen, W. L.; Hudson, M. R.; Planas, N.; Borycz, J.; Dzubak, A. L.; Verma, P.; Lee, K.; Bonino, F.; Crocellà, V.; Yano, J.; Bordiga, S.; Truhlar, D. G.; Gagliardi, L.; Brown, C. M.; Long, J. R. “Oxidation of Ethane to Ethanol by N2O in a Metal–Organic Framework with Coordinatively Unsaturated Iron(II) Sites.” *Nature Chemistry* (6), 2014; pp. 590–595. Available at: http://www.nature.com/nchem/journal/v6/n7/full/nchem.1956.html.

[16] In addition to JCAP and CASL, a third hub, the Energy Efficient Buildings (EEB) Hub, was stood up in 2009. However, the scope of work and funding level was reduced in 2014, and the Hub classification was removed to reflect this change. The research center was renamed the Consortium for Building Energy Innovation (CBEI) and has been integrated into the main DOE-EERE program. It is currently developing technology systems to improve energy efficiency in existing small- and medium-sized commercial buildings. Led by Pennsylvania State University, CBEI brings together fourteen organizations from universities, DOE national laboratories, and the private sector. For more information, see http://cbei.psu.edu/.

[17] JCAP and CASL were initially awarded up to $122 million over five years, while CMI and JCESR were initially awarded up to $120 million over five years (subject to appropriations). In 2015, JCAP was renewed at up to $75 million over five years, and CASL was renewed up to $121.5 million over five years (pending congressional approval). In contrast, the first set of forty-six EFRCs, initiated in 2009, was funded at the level of $2–$5 million per year per center for five years. The second set of EFRCs, started in 2014, are funded at the level of $2–$4 million per year per center for four years, with an average award of $3.125 million per year per center (32 EFRCs, $100 million total program funding per year, subject to appropriations).

[18] For example, there is currently no industrial solar fuels production. JCAP is therefore coordinating R&D across many research laboratories, including multiple EFRCs, to accelerate the pace of technology development and realize an entirely new direct solar fuels industry. By comparison, JCESR and CMI are striving to create new technologies that have the potential to transform large, established industries. They work closely with industrial partners as well as EFRCs (in the case of JCESR) to guide research efforts and ensure practical solutions that are competitive in marketplaces.

[19] See textbox: Joint Center for Artificial Photosynthesis , in Chapter 7 (“Advancing Systems and Technologies to Produce Cleaner Fuels”) and http://www.solarfuelshub.org.

[20] For more on the Joint Center for Energy Storage Research, see text box in Chapter 8 (“Advancing Clean Transportation and Vehicle Systems and Technology”) and http://www.jcesr.org/.

[21] CASL research is also supported by the SC-ASCR program through expertise in HPC and dedicated allocation on Titan, one of two DOE-SC leadership-class computing user facilities (see Section 9.6.1). For more on CASL, see http://www.casl.gov/.

[22] The criticality of selected rare earth metals as well as other elements used in clean energy technology and components was reviewed in the 2011 “Critical Materials Strategy” report; see http://energy.gov/node/349057. More on this topic is included in Chapter 6, “Innovating Clean Energy Technologies in Advanced Manufacturing.”

[23] For more on CMI, see http://www.cmi.ameslab.gov.

[24] Hu, S.; Shaner, M. R.; Beardslee, J. A.; Lichterman, M.; Brunschwig, B. S.; Lewis, N. S. “Amorphous TiO2 Coatings Stabilize Si, GaAs, and GaP Photoanodes for Efficient Water Oxidation.” *Science* (344), 2014; pp. 1005-1009. Available at: http://www.sciencemag.org/content/344/6187/1005.full?sid=4756f1a2-32db-40e6-ae85-dc503655658e.

[25] The three BRCs are the Bioenergy Science Center at ORNL, the Great Lakes Bioenergy Research Center at the University of Wisconsin-Madison, and the Joint Bioenergy Institute at LBNL. See Fundamental Research: Bioenergy Research Centers textbox in Chapter 7, “Advancing Systems and Technologies to Produce Cleaner Fuels.”

[26] The scientific rationale for the three BRCs and for fundamental genomic research for biofuels and bioproducts was established by the 2005 workshop Biomass to Biofuels, which is summarized in the report “Breaking the Biological Barriers to Cellulosic Ethanol: A Joint Research Agenda.” DOE/SC-0095. Washington, DC: U.S. Department of Energy Office of Science. Available at: http://www.genomicscience.energy.gov/biofuels/b2bworkshop.shtml.

[27] The three BRCs are funded at $25M per center per year for up to five years (pending congressional approval). The three BRCs were renewed for a second five-year phase in 2012.

[28] From 2008 to 2013, the three BRCs published nearly 1,350 papers in peer-reviewed journals.

[29] From 2008 to 2013, the three BRCs disclosed 325 inventions and filed 176 patent applications of which 72 were licensed/optioned. A chart of cumulative totals by year from 2008 to 2013, the full list of BRC partners, and examples of recent technology transfer to the private sector are included in Bioenergy Research Centers, U.S. DOE, Office of Science, Office of Biological and Environmental Research, February 2014. Available at: http://genomicscience.energy.gov/centers/BRCs2014HR.pdf.

[30] Ibid.

[31] Transcriptomics is the study of the transcriptome, which is defined as the complete set of RNA transcripts produced by a genome, using high-throughput (or -omics) techniques. This definition is derived from http://www.nature.com/subjects/transcriptomics.

[32] Foo; J. L.; Jensen, H. M.; Dahl, R. H.; George, K.; Keasling, J. D.; Lee, T. S.; Leong, S.; Mukhopadhyay, A. "Improving Microbial Biogasoline Production in *Escherichia coli Using Tolerance Engineering*." *MBio* (5:6), 2014; pp. e01932-e01914. Available at: http://mbio.asm.org/content/5/6/e01932-14.

[33] DOE-designated user facilities are also critically important for basic research in the biological and medical sciences and for national security.

[34] An interactive map of DOE-SC scientific user facility statistics for FY 2014, as well as the source data, is available at http://science.energy.gov/user-facilities/user-statistics/. This interactive map provides information on individual user projects at each facility, including institutional affiliation, number of users from that institution, and congressional district of the institution. More information on scientific user facility usage is provided in Supplemental Information (section 9C.

[35] Detailed information on the types of agreements available to potential users of DOE designated user facilities is available at http://energy.gov/gc/access-high-technology-user-facilities-doe-national-laboratories. All DOE-SC scientific user facilities are open access to interested users as defined in a 2012 DOE-SC memorandum available at http://science.energy.gov/~/media/_/pdf/user-facilities/memoranda/Office_of_Science_User_Facility_Definition_Memo.pdf. Additional information about DOE-SC scientific user facility policies is available at http://science.energy.gov/user-facilities/frequently-asked-questions/.

[36] For examples of the diversity of science and technology research at the multipurpose user facilities, see the APS Science 2014 brochure at https://www1.aps.anl.gov/files/download/APS-Science/APS_Science_2014.pdf; the ORNL Neutron Sciences division Strategic Plan 2014 at https://neutrons.ornl.gov/sites/default/files/NScD-Strategic-Plan-2014.pdf; and the five-year strategic plans for The Molecular Foundry at http://foundry.lbl.gov/assets/docs/TMF-Strategic-Plan.pdf and the Center for Functional Nanomaterials at https://www.bnl.gov/cfn/strategicplan/mission.php. For more on the research diversity at EMSL, see Section 9.5.2 and references therein. For more on the research diversity of the high-performance computing facilities supported by the DOE-SC, see Section 9.6.1 and references therein.

[37] For example, the five X-ray light sources stewarded by the SC-BES program are an invaluable tool for the biological sciences, providing unique capabilities for characterizing biological molecules from single protein crystals to imaging of whole cells. At LCLS, while about 50% of the nearly 600 users are from the physics community, more than a quarter of users are from the biological and chemical sciences.

[38] The Energy Systems Integration Facility is maintained by DOE-EERE and the National Renewable Energy Laboratory. More information is available at http://www.nrel.gov/esif/.

[39] For more information on the Advanced Test Reactor and other capabilities in the NSUF, see http://www4vip.inl.gov/research/advanced-test-reactor-research/.

[40] The Carbon Fiber Technology Facility houses a highly instrumented carbon fiber production line for demonstrating scalability to near production-scale. More information is available at http://www.ornl.gov/user-facilities/cftf.

[41] Additional information on MDF capabilities, research projects, and partnering organizations is available at http://web.ornl.gov/sci/manufacturing/.

[42] A complete list of the experimental capabilities available at the Building Envelope, Building Technology, and System/Building Integration Centers of Excellence is described in the "Experimental Capabilities & Apparatus Directory," available at http://web.ornl.gov/sci/buildings/docs/buildings_catalog.pdf.

[43] Experimental capabilities include dynamometers (for engines, motors, and vehicles), analytical chemistry and catalysis laboratories, in situ chemical speciation for catalysts and engines (methods invented at ORNL), power electronic and electric motor device testing, battery manufacturing, and the Vehicle Systems Laboratory, containing a full powertrain research cell suitable for studying class 8 truck systems. A complete list of capabilities is available at http://web.ornl.gov/sci/transportation/facilities/ntrc/index.shtml.

[44] The Sustainable Transportation Program's strategy includes accelerating electric vehicle penetration, increasing all vehicle efficiency through lighter materials, hybrid drives and advanced combustion technology, adoption of renewable biofuels and natural gas, and decision science. More is available in the Sustainable Transportation Program brochure at http://web.ornl.gov/sci/transportation/docs/brochures/STP-Brochure.pdf.

[45] More information is available at https://www.inl.gov/wnuf/.

[46] Acronyms used in Table 9.1 are as follows: (1) Department of Energy Office of Energy Efficiency and Renewable Energy (DOE-EERE), (2) Office of Nuclear Energy (DOE-NE), (3) Office of Basic Energy Sciences (SC-BES), (4) Office of Biological and Environmental Research (SC-BER), (5) Office of Advanced Scientific Computing Research (SC-ASCR), (6) Office of High Energy Physics (SC-HEP), (7) Office of Nuclear Physics (SC-NP), and (8) Office of Fusion Energy Science (SC-FES).

[47] In the FY 2016 budget request, the DOE-SC has proposed that this will be the final year of funding support for the Alcator C-Mod facility.

[48] Acronyms and shortened forms used in Table 9.2 are as follows: (1) Ames Laboratory (Ames), (2) Argonne National Laboratory (ANL), (3) Brookhaven National Laboratory (BNL), (4) Fermi National Accelerator Laboratory (FNAL), (5) Idaho National Laboratory (INL), (6) Lawrence Berkeley National Laboratory (LBNL), (7) National Energy Technology Laboratory (NETL), (8) National Renewable Energy Laboratory (NREL), (9) Oak Ridge National Laboratory (ORNL), (10) Pacific Northwest National Laboratory (PNNL), and (11) Sandia National Laboratories (SNL).

[49] Examples include the Battery Test Facilities at ANL, the Facility for Low Energy Experiments in Buildings (FLEXLAB) and the Advanced Biofuels Processing Demonstration Unit (ABPDU) at LBNL, and the National Solar Thermal Test Facility at SNL.

[50] The Combustion Research Facility at SNL is a joint DOE-SC and DOE-EERE facility dedicated to combustion science and technology. Users have access to capabilities ranging from flame analysis to laser-based in cylinder process characterization. The National Transportation Research Center at ORNL supports the private sector and government agencies in development of advanced vehicle technologies. Available capabilities range from analytical laboratories for catalysis and combustion to the vehicle systems laboratory, a full powertrain research cell large enough for class 8 truck systems.

[51] Examples include the materials preparation center at Ames and the high throughput facility for materials chemistry development at ANL.

[52] A complete, searchable list of DOE designated user facilities and shared R&D facilities, including Web links, is available at http://energy.gov/technologytransitions/technology-transitions-facilities-database.

[53] Work at laboratory R&D facilities will typically be supported by technology partnership agreements (Collaborative Research and Development Agreements [CRADA] or Strategic Partnership Projects [SPP; formerly known as Work for Others]). The facilities at the National Energy Technology Laboratory are made available to researchers through an alternative contractual mechanism. More information on this and other access agreements can be found at http://energy.gov/technologytransitions/technology-transitions-facilities-database.

[54] Savee, J. D.; Papajak, E.; Rotavera, B.; Huang, H.; Eskola, A. J.; Welz, O.; Sheps, L.; Taatjes, C. A.; Zádor, J.; Osborn, D. L. "Direct Observation and Kinetics of a Hydroperoxyalkyl Radical (QOOH)." Science (347:6222), 2015; pp. 643-646. Available at: http://www.sciencemag.org/content/347/6222/643.full?sid=0f7b894c-d4ae-4026-8758-6bfaf9b2e7ce.

[55] "From Quanta to the Continuum: Opportunities for Mesoscale Science." A report from the Basic Energy Sciences Advisory Committee, September 2012. Available at: http://science.energy.gov/~/media/bes/pdf/reports/files/OFMS_rpt.pdf.

[56] Ibid.

[57] For more on the properties of synchrotron radiation and the types of experiments it enables, see "Experimental Techniques at Light-source Beamlines." Available at: http://science.energy.gov/~/media/bes/pdf/Synchrotron_Techniques.pdf.

[58] More information on the technical specifications of each X-ray light source, as well as complete listings of experiments available, can be found at the facility Web sites.

[59] Recent examples from the national laboratories are as follows: (a) Liu, H.; Strobridge, F. C.; Borkiewicz, O. J.; Wiaderek, K. M.; Chapman, K. W.; Chupas, P. J.; Grey, C. P. "Capturing Metastable Structures During High-rate Cycling of LiFePO4 Nanoparticle Electrodes." *Science* (344:6191), 2014; pp. 1252817-1-7. Available at: http://www.sciencemag.org/content/344/6191/1252817 (APS). (b) Liu, X. S.; Wang, D. D.; Liu, G.; Srinivasan, V.; Liu, Z.; Hussain, Z.; Yang, W. L. "Distinct Charge Dynamics in Battery Electrodes Revealed by In Situ and Operando Soft X-ray Spectroscopy." *Nature Communications* (4), 2013. Available at: http://www.nature.com/ncomms/2013/131008/ncomms3568/full/ncomms3568.html (ALS). (c) Yu, Y-S.; Kim, C.; Liu, Y.; Van der Ven, A.; Meng, Y. S.; Kostecki, R.; Cabana, J. "Nonequilibrium Pathways During Electrochemical Phase Transformations in Single Crystals Revealed by Dynamic Chemical Imaging at Nanoscale Resolution." *Advanced Energy Materials* (5:7), 2015. Available at: http://onlinelibrary.wiley.com/doi/10.1002/aenm.201402040/abstract (SSRL).

[60] Wang, Y.; Liu, X.; Im, K-S.; Lee, W-K.; Wang, J.; Fezzaa, K.; Hung, D. L. S.; Winkelman, J. R. "Ultrafast X-ray Study of Dense-liquid-jet Flow Dynamics Using Structure-tracking Velocimetry." *Nature Physics* (4), 2008; pp. 305-309. Available at: http://www.nature.com/nphys/journal/v4/n4/abs/nphys840.html.

[61] The Solar Shingle is a commercial product developed by Dow Chemical Company that integrates a series of small form factor photovoltaic devices directly into roofing material. In situ X-ray diffraction and scanning techniques were used at the APS to develop a semiconductor fabrication process that would optimize the solar photovoltaic properties of the CIGS active material. For more on the solar shingle developed by Dow Chemical Company, see Supplemental Information (section 9D).

[62] The prizes include the 2012 prize for studies of the G-protein coupled receptors (Advanced Photon Source); the 2009 prize for the structure of the ribosome (National Synchrotron Light Source); the 2008 prize for green fluorescent protein (National Synchrotron Light Source); and the 2006 prize for DNA transcription (Stanford Synchrotron Radiation Light Source). A fifth prize in 2002 was awarded for the study of ion channels in cell membranes (National Synchrotron Light Source).

[63] In addition to the five X-ray light sources currently operating in the United States, there are currently eight operating storage rings and free electron lasers in Europe and Asia. Next generation storage rings are in development in Brazil, France, Germany, Japan, and Sweden, and hard X-ray FELs (similar to LCLS) are under construction in Germany, Korea, and Switzerland. More information on the international light sources, including comparative technical information, is available in the 2013 BESAC report, "Future X-ray Light Sources." Available at: http://science.energy.gov/bes/besac/reports/.

[64] The scientific basis for the upgrades to LCLS and APS (LCLS-II and APS-U, respectively) are presented in the 2013 BESAC report, "Future X-ray Light Sources." Available at: http://science.energy.gov/bes/besac/reports/.

[65] When fully built out, NSLS-II will accommodate 60–70 beamlines. Descriptions of the beamlines available and a timeline for development of new beamlines (with links to associated projects and beamline descriptions) are available at http://www.bnl.gov/ps/nsls2/beamlines/timeline.php.

[66] Öström, H.; Oberg, H.; Xin, H.; LaRue, J.; Beye, M.; Dell'Angela, M.; Gladh, J.; Ng, M. L.; Sellberg, J. A.; Kaya, S.; Mercurio, G.; Nordlund, D.; Hantsschmann, M.; Hieke, F.; Kühn, D.; Schlotter, W. F.; Dakovski, G. L.; Turner, J. J.; Minitti, M. P.; Mitra, A.; Moeller, S. P.; Föhlisch, A.; Wolf, M.; Wurth, W.; Persson, M.; Nørskov, J. K.; Abild-Pedersen, F.; Ogasawara, H.; Pettersson, L. G. M.; Nilsson A. "Probing the Transition State Region in Catalytic CO Oxidation on Ru." *Science* (347:6225), 2015; pp. 978-982. Available at: http://www.sciencemag.org/content/347/6225/978.full?sid=a9fb4930-933b-4778-b609-1cbd9c367567.

[67] The SNS and HFIR user facilities hosted approximately 1,350 unique users in FY 2014.

[68] Spallation is a process by which neutrons and other particles are ejected from a heavy metal target owing to impacts from a high-energy particle beam. At the Spallation Neutron Source at Oak Ridge National Laboratory, neutrons are produced by the spallation process from a liquid mercury target in a beam of protons from a linear accelerator operating in a 60 Hz pulse mode at 1 GeV and at a power level of approximately 1.4 MW.

[69] The High Flux Isotope Reactor produces a continuous beam of neutrons from a light-water moderated and cooled nuclear reactor operating at 85 MW. The HFIR provides neutrons to a full suite of instruments, including diffraction, small angle scattering, imaging, and inelastic scattering. A complete list of experiments with links to descriptions and scientific applications is available at https://neutrons.ornl.gov/hfir.

[70] Each scattering instrument is tailored for specific types of scattering experiments, including diffraction, reflectometry, inelastic scattering, and small angle scattering. A list of SNS experiments and links to descriptions, including scientific applications, is available at https://neutrons.ornl.gov/sns.

[71] Neutron scattering has been used to study stresses in jet engine turbines, bridge support cables, and additive manufacturing processes. These and other examples are summarized at https://neutrons.ornl.gov/ and in the included scientific references.

[72] Because the energy of the moderated neutrons is in the milli-electron volt range, comparable to that of quantized elementary atomic and magnetic excitations (phonons and magnons), the interaction of the neutron in passing through the sample can excite or de-excite these elementary excitations, thereby driving a corresponding shift in the energy of the scattered neutrons. This energy shift can be measured by the spectrometer and provides information about the excitation.

[73] The National Institute of Standards and Technology Center for Neutron Research provides cold and thermal neutrons to a broad suite of instruments for all qualified applicants from universities, the private sector, and other government agencies. NCNR is a user facility operated by the U.S. Department of Commerce. More can be found at https://www.ncnr.nist.gov/.

[74] In addition to the two domestic sources, there are multiple neutron sources operating or in development internationally. For example, the Japanese J-Parc facility is a one megawatt class pulse neutron facility offering a comprehensive suite of instruments via a user program. The Institut Laue-Langevin (ILL) in Grenoble, France, is the world's highest flux continuous wave neutron source. When complete, the European Spallation Source in Lund, Sweden will be the world's most advanced neutron source, operating at five megawatts and providing the largest number of instruments at the highest neutron flux. Operation is expected to begin in 2019.

[75] The scientific drivers and user demand for these capabilities were delineated by a series of user-led workshops in 2014. The proposed technical details and applications of the second target station are described in the 2013 BESAC report "Basic Energy Sciences Facilities Prioritization." Available at: http://science.energy.gov/~/media/bes/besac/pdf/Reports/BESAC_Facilities_Prioritization_Report_2013.pdf.

[76] Nanoscience Research for Energy Needs, BES-cosponsored NNI Workshop, March 16–18, 2004.

[77] The NSRC Program is a major component of the DOE-SC contribution to the NNI. Additional support for nanoscale science and engineering research within DOE is provided by the offices of DOE-EERE, DOE-FE, and DOE-NE. More on the DOE involvement with the NNI is available at www.science.energy.gov/bes/research/national-nanotechnology-initiative. NNI involves 20 departments and agencies that collaborate toward "a future in which the ability to understand and control matter at the nanoscale leads to a revolution in technology and industry that benefits society." More on the National Nanotechnology Initiative is available at http://www.nano.gov.

[78] Descriptions of each NSRC, as well as other colocated user facilities, are provided at http://science.energy.gov/bes/suf/user-facilities/nanoscale-science-research-centers/.

[79] A more comprehensive list of the specialties available at the five NSRCs across the categories of synthesis, characterization, and theory/modeling/simulation can be found at the NSRC Portal hosted by SNL. Available at: https://nsrcportal.sandia.gov.

[80] Industrial activities at the NSRCs range from basic to applied research, conducted by both small start-up and large, established corporations. Many examples of recent industrial research projects at the NSRCs are described at https://nsrcportal.sandia.gov/home/industrial.

[81] For more on the impact of nanotechnology for energy applications, see the brochure "Nanotechnology and Energy: Powerful Things from a Tiny World." Available at: http://www.nano.gov/node/734. For more on the benefits and applications of nanoscience, see http://www.nano.gov/you/nanotechnology-benefits.

[82] (a) Llordes, A.; Garcia, G.; Gazquez, J.; Milliron, D. J. "Tunable near-infrared and visible light transmittance in nanocrystal-in-glass composites." *Nature* (500), 2013; pp. 323-326. Available at: http://www.nature.com/nature/journal/v500/n7462/full/nature12398.html. (b) Runnerstrom, E. L.; Llordes, A.; Lounis, S. D.; Milliron, D. J. "Nanostructured Electrochromic Smart Windows: Traditional Materials and NIR-selective Plasmonic Nanocrystals." *Chemical Communications* (50:73), 2014; pp. 10555-10572. Available at: http://pubs.rsc.org/en/content/articlelanding/2014/cc/c4cc03109a.

[83] Demortière, A.; Snezhko, A.; Sapozhnikov, M. V.; Becker, N.; Proslier, T.; Aranson, I. S. "Self-Assembled Tunable Networks of Sticky Colloidal Particles." *Nature Communications* (5), 2014. Available at: http://www.nature.com/ncomms/2014/140121/ncomms4117/full/ncomms4117.html.

[84] The DOE Systems Biology Knowledgebase (KBase, http://kbase.us) is a large-scale bioinformatics system supporting the BER genomic science user community. KBase allows users to upload, analyze, and model their data as well as share workflows and conclusions with the broader community. The data collected through routine operations and scientific field experiments at ARM are stored at the ARM data archive and made publically available to registered users at http://www.archive.arm.gov.

[85] JGI was originally established in 1997 to support the DOE role in the Human Genome Project. JGI united the expertise and resources in DNA sequencing, informatics, and technology development that existed in the three DOE genome centers at LBNL, LANL, and LLNL. LBNL, as lead laboratory, consolidated activities at the current location in Walnut Creek, CA. This enabled a dramatic increase in the scale of JGI activities.

[86] JGI data is freely available to registered users at the DOE JGI Genome Portal, http://jgi.doe.gov/data-and-tools. Additionally, users have access to more specialized data and analysis resources, including the Integrated Microbial Genomes, Integrated Microbial Genome/Metagenomes, and the Phytozome, Mycocosm, and Genomes On-line Database.

[87] More on the BRCs is available in Section 9.2.3 of this chapter and in Chapter 7, "Advancing Systems and Technologies to Produce Cleaner Fuels."

[88] Biofuels currently provide approximately 5% of total U.S. energy supply, primarily in the transportation sector. For more information see Chapter 7, "Advancing Systems and Technologies to Produce Cleaner Fuels."

[89] The report "Biomass as Feedstock for a Bioenergy and Bioproducts Industry: The Technical Feasibility of a Billion-Ton Annual Supply" (the Billion-Ton Study or 2005 BTS) was conducted in 2005 to determine the potential domestic capacity of biomass for energy. A follow-up study, "U.S. Billion Ton Update: Biomass Supply for Bioenergy and Bioproducts Industry" (or 2011 BT2), was completed in 2011. Both reports are available at https://bioenergykdf.net/content/billiontonupdate.

[90] The current 10-year JGI strategic vision (http://jgi.doe.gov/wp-content/uploads/2013/05/10-Year-JGI-Strategic-Vision.pdf) was assembled with extensive input from DOE, JGI users, and advisory panels. The plan describes key scientific goals that need to be addressed and outlines a portfolio of new strategic capabilities to be developed over the next decade to enable users of the facility to achieve these goals.

[91] Available at: http://www.jgi.doe.gov/programs/GEBA/.

[92] Rinke, C.; Schwientek, P.; Sczyrba, A.; Ivanova, N. N.; Anderson, I. J.; Cheng, J-F.; Darling, A.; Malfatti, S.; Swan, B. K.; Gies, E. A.; Dodsworth, J. A.; Hedlund, B. P.; Tsiamis, G.; Sievert, S. M.; Liu, W-T.; Eisen, J. A.; Hallam, S. J.; Kyrpides, N. C.; Stepanauskas, R.; Rubin, E. M.; Hugenholtz, P.; Woyke T. "Insights into the Phylogeny and Coding Potential of Microbial Dark Matter." *Nature* (499), 2013; pp. 431–437. Available at: http://www.nature.com/nature/journal/v499/n7459/full/nature12352.html.

[93] The scope of EMSL as originally defined by former PNNL director William Wiley was, in part, a response to the 1985 National Academy of Sciences report "Opportunities in Chemistry." Available at: http://www.nap.edu/catalog/606/opportunities-in-chemistry.

[94] A description of the major capabilities provided to users of the EMSL is available at https://www.emsl.pnl.gov/emslweb/scientific-capabilities.

[95] The Biosystems Dynamics and Design program is focused on regulation of spatial and temporal parameters of metabolic processes in plants, fungi, and microbes. The overarching goal is to understand how biological systems respond to and modify their environment and ultimately to modify and manipulate these systems for novel bioenergy and biorenewable technologies. For specific capabilities and recent science highlights from the Biosystems Dynamics and Design program, see https://www.emsl.pnl.gov/emslweb/science/biosystem.

[96] The Terrestrial and Subsurface Ecosystems program couples experimentally derived mechanistic understanding of biogeochemical and microbial processes in the environment with pore-scale hydrological models to improve strategies for sustainable contaminant remediation, attenuation, and biogeochemical cycling. For specific capabilities and recent science highlights from the Terrestrial and Subsurface Ecosystems program, see http://www.emsl.pnl.gov/emslweb/science/terrestrial.

[97] The Energy Materials and Systems program focuses on facilitating the development and dissemination of molecular-level understanding and predictive modeling of interfaces to enable the design and development of efficient and environmentally benign energy storage and conversion systems. For specific capabilities and recent science highlights, see http://www.emsl.pnl.gov/emslweb/science/energy.

[98] The tesla is the international system of units' measure of magnetic flux density. The 21 Tesla magnet in this instrument enables users to gain unprecedented mass resolution and accuracy, with mass measurements possible to five to six decimal points and accuracy to one part-per-million. The high mass resolution provided allows definitive identification of all molecular species in a complex system, while the high mass accuracy will help remove ambiguity in identifying molecular species. The scientific basis for development of the 21 Tesla high-resolution mass accuracy capability was delineated by a workshop held in 2008. Available at: http://www.emsl.pnl.gov/emslweb/next-generation-mass-spectrometry. More information on this system is available at http://www.emsl.pnl.gov/emslweb/21t-high-resolution-mass-accuracy-capability.

[99] Knopf, D. A.; Alpert, P. A.; Wang, B.; O'Brien, R. E.; Kelly, S. T.; Laskin, A.; Gilles, M. K.; Moffet, R. C. "Microspectroscopic Imaging and Characterization of Individually Identified Ice Nucleating Particles from a Case Field Study." *Journal of Geophysical Research—Atmospheres* (119:17), 2014; pp. 10,365-10,381. Available at: http://onlinelibrary.wiley.com/doi/10.1002/2014JD021866/full.

[100] ARM is managed and operated by nine DOE national laboratories. Each laboratory has specific roles and responsibilities in the partnership. For a list of the partnering labs and their responsibilities in the ARM program, see http://www.arm.gov/about/organization/labs.

[101] Since 2005, ARM mobile sites have been deployed in North and South America, Europe, Asia, and Africa.

[102] The ARM aerial facility provides airborne measurements to address ARM science questions by using either external aircraft or the DOE-supported Gulfstream-1 and Cessna 206 aircraft. The aerial facility includes multiple aircraft sensors for in situ measurements of atmospheric, aerosol, and cloud properties. Available at: http://www.arm.gov/sites/aaf.

[103] Remote sensing instruments available at ARM sites include vertically pointing and scanning radars, lidars, and multiple radiometers. For a complete list of measurement capabilities at each ARM site, see http://www.arm.gov/instruments.

[104] These observations have led to improvements in temperature and humidity profiles as well as cloud amount in the middle and upper troposphere. For this and other applications of ARM data, see "Contributions of the Atmospheric Radiation Measurement (ARM) Program and the ARM Climate Research Facility to the U.S. Climate Change Science Program." September 2008. Available at: http://www.arm.gov/publications/programdocs/doe-sc-arm-0803.pdf?id=61.

[105] The ARM data archive is located at http://www.archive.arm.gov/armlogin/login.jsp.

[106] The 983 users of ARM in FY 2014 represent universities, the private sector, DOE national laboratories, other federal agencies, and international institutions.

[107] Feldman, D. R.; Collins, W. D.; Gero, P. J.; Torn, M. S.; Mlawer, E. J.; Shippert T. R. “Observational Determination of Surface Radiative Forcing by CO2 from 2000 to 2010.” *Nature* (519), 2015; pp. 339-343.

[108] http://www.nap.edu/catalog/18805/climate-intervention-carbon-dioxide-removal-and-reliable-sequestration.

[109] http://www.nap.edu/catalog/18988/climate-intervention-reflecting-sunlight-to-cool-earth.

[110] The Materials Project at LBNL (see http://www.materialsproject.org) combines supercomputing at NERSC (see Section 9.6.1) with novel electronic structure calculation methods to calculate properties of known and predicted materials as well as provide tools for designing novel materials with tailored properties.

[111] CASL, a DOE Energy Innovation Hub, has developed modeling and simulation tools for nuclear reactor behavior at unprecedented fidelity. These tools have been optimized to leverage the computing power of Titan, a DOE leadership-class computer at ORNL (see Section 9.6.1).

[112] A team from SNL utilized Titan to perform direct numerical simulation to simulate a jet flame burning dimethyl ether. The resulting improvement to models based on these results will be used in engineering-scale computational fluid dynamics simulations that are used to optimize combustion devices burning a variety of fuels with the ultimate goal of shortening the design lifetime for new technology. For more information see “The Complexities of Combustion” at https://www.olcf.ornl.gov/2014/11/11/the-complexities-of-combustion/ and references therein.

[113] In collaboration with ORNL, BMI Corporation engineers leverage the computing capabilities of Titan to study air flow around class 8 long-haul trucks and optimize add-on parts that could dramatically reduce drag. The resulting UnderTray system, marketed by SmartTruck Systems, can improve fuel efficiency by more than 10%. Leveraging DOE high-performance computers, BMI Corporation was able to reduce the time from concept to manufacture-ready design from three years to 18 months.

[114] GE Global Research have used Titan at ORNL to model the formation of ice on various ice-phobic surfaces in an effort to reduce the energy cost of maintaining ice-free turbine blades and promote development of wind resources in colder climates. For more information, see “Titan Propels GE Wind Turbine Research into New Territory” at https://www.olcf.ornl.gov/2013/10/25/titan-propels-ge-wind-turbine-research-into-new-territory/ and references therein.

[115] Relevant workshops and associated reports are tabulated in Supplemental Information (Chapter 1). A list with brief descriptions of the workshop scope is available at http://science.energy.gov/ascr/news-and-resources/workshops-and-conferences/ (from 2014 on) and http://science.energy.gov/ascr/news-and-resources/workshops-and-conferences/workshops-conferences-archive/ (from 2006 to 2013).

[116] See Section 9.6.1 for more information on the INCITE and ALCC funding programs.

[117] Recent industrial projects leveraging Office of Science computing resources are tabulated in Supplemental Information (section 9B).

[118] For more on CASL see textbox, “Westinghouse–CASL Team Simulates High-Fidelity Next-Generation Light Water Reactors” in Section 9.6.3.

[119] The Advanced Computing Tech Team (ACTT) is comprised of representation from the DOE energy technology offices, DOE-SC, NNSA, and DOE national laboratories. Its goal is to deliver technologies that will be used to create new scientific insights into complex physical systems. The ACTT serves as a mechanism by which DOE programs working in the HPC space can communicate their efforts and identify new, mutually beneficial opportunities. These efforts have led to multiple workshops engaging with external stakeholders. More on the ACTT can be found at http://www.energy.gov/advanced-computing-tech-team.

[120] Supercomputer performance is typically described in terms of the number of petaflops (pflops), or $1x10^{15}$ floating-point operations per second (FLOPS). The threshold for exascale computing is defined as 1,000 pflops. For comparison, current DOE leadership-class computers are between 8 and 18 pflops.

[121] For comparison, seven of the top fifteen supercomputers are located in Europe and Asia.

[122] FLOPS or flops (FLoating-point Operations Per Second) is a measure of a computer’s performance.

[123] Examples of leadership-class computing research from FY 2015 are tabulated in Supplemental Information (section 9B).

[124] Bayerl, D.; Kioupakis, E. “Visible-Wavelength Polarized-Light Emission with Small-Diameter InN Nanowires.” *Nano Letters* (14:7), 2014; pp. 3709-3714. Available at: http://pubs.acs.org/doi/pdf/10.1021/nl404414r.

[125] The availability of these machines is based on the DOE High-end Computing Act of 2004.

[126] In 2015, the ALCC provided 2.9 billion hours of computational time to 43 research projects that had already received federal, state, or corporate funding. The total requested hours were 10.7 billion hours, indicating these facilities are oversubscribed by a factor of 3.7.

[127] In FY 2015, INCITE has allocated 3,670 million core hours to 37 projects. Twelve projects, accounting for 1,322 core hours, having relevance to the technologies surveyed in the QTR, are tabulated in Supplemental Information (section 9B). Note that INCITE projects are not required to be immediate DOE research priorities.

[128] Constable, G.; Somerville, B. *A Century of Innovation: Twenty Engineering Achievements that Transformed our Lives*. National Academies Press, Washington, DC, 2003.

[129] Ela, E.; Milligan, M.; Kirby, B. “Operating Reserves and Variable Generation.” NREL/TP-5500-51978, August 2011. Available at: http://www.nrel.gov/docs/fy11osti/51978.pdf.

[130] (a) Petra, C. G.; Schenk, O.; Anitescu, M. "Real-time Stochastic Optimization of Complex Energy Systems on High Performance Computers." *Computing in Science and Engineering* (16:5), 2014; pp. 32-42. Available at: http://ieeexplore.ieee.org/xpl/articleDetails.jsp?arnumber=6809706. (b) Constantinescu, E.; Zavala, V.; Rocklin, M.; Lee, S.; Anitescu, M. "A Computational Framework for Uncertainty Quantification and Stochastic Optimization in Unit Commitment with Wind Power Generation." *IEEE Transactions on Power Systems* (26:1), 2011; pp. 431-441. Available at: http://ieeexplore.ieee.org/xpl/articleDetails.jsp?arnumber=5467169. (c) Lubin, M.; Petra, C. G.; Anitescu, M.; Zavala, V. "Scalable Stochastic Optimization of Complex Energy Systems." SC11 Proceedings of 2011 International Conference for High Performance Computing, Networking, Storage and Analysis, November 12–18, 2011, Seattle, Washington. ANL/MCS-P1858-0311. Argonne, IL: Argonne National Laboratory, 2011. Available at: http://www.mcs.anl.gov/publication/scalable-stochastic-optimization-complex-energy-systems.

[131] For more information, see http://www.mcs.anl.gov/MACS/.

[132] "National Power Grid Simulation Capability: Needs and Issues." U.S. Department of Homeland Security, Science and Technology Directorate, 2008.

[133] Complete lists of private sector allocations for FY 2015 at OLCF, ALCF, and NERSC are tabulated in Supplemental Information (section 9B).

[134] Grosvenor, A. D.; Rixon, G. S.; Sailer, L. M.; Matheson, M. A.; Gutzwiller, D. P.; Demeulenaere, A.; Contier, M.; Strazisar, A. J. "High Resolution RANS NLH Study of Stage 67 Tip Injection Physics." ASME Turbo Expo 2014: Turbine Technical Conference and Exposition; June 16–20, 2014, Düsseldorf, Germany. Paper No. GT2014-27219, p. V02BT39A045.

[135] A table of the high-performance computers sited at DOE national laboratories that rank in the top 150 fastest computers is provided in Supplemental Information (section 9B).

[136] "Case Study: Plexos and Power Modeling Software." High Performance Computing Innovation Center. Accessed June 12, 2015: http://hpcinnovationcenter.llnl.gov/case-study-plexos-and-power-modeling-software.

[137] "Case Study: Navistar and Semi-Truck Fuel Efficiency." High Performance Computing Innovation Center. Accessed June 12, 2015: http://hpcinnovationcenter.llnl.gov/case-study-navistar-and-semi-truck-fuel-efficiency.

[138] The High Performance Computing Center housed in the Energy Systems Integration Facility at NREL hosts Peregrine, a 1.2 pflop (peak performance) computer dedicated to renewable energy and energy efficiency research. More information is available at http://hpc.nrel.gov/about.

[139] The High Performance Computer for Energy and the Environment (HPCEE) is a 0.503 pflop computer housed in the Simulation-based Engineering User Center at the National Energy Technology Laboratory (NETL). More information is available at https://hpc.netl.doe.gov/.

[140] http://energy.gov/articles/department-energy-awards-425-million-next-generation-supercomputing-technologies.

[141] A complete map of ESNet is available at https://www.es.net/engineering-services/the-network/.

[142] Examples include Trilinos (SNL), PETSc (ANL), and Chombo (LBNL).

[143] For more on Energy Innovation Hubs, see Section 9.2.2.

[144] Franceschini, F.; Oelrich, Jr., B.; Gehin, J. "Simulation of AP1000 First Core with VERA." *Nuclear Engineering International*, 2014; pp. 33-35. Available at: http://www.neimagazine.com/features/featuresimulation-of-ap1000-first-core-with-vera-4295660/.

[145] Of the more than 300 alumni of the program, 28% are in government, 38% in education, and 34% in the private sector.

[146] The benefits of exascale and the scope of the challenge in reaching this level of computing were laid out in the 2010 ASCAC report "The Opportunities and Challenges of Exascale Computing." Available at: http://science.energy.gov/~/media/ascr/ascac/pdf/reports/Exascale_subcommittee_report.pdf.

[147] *A National Strategy for Advancing Climate Modeling*. The National Academies, 2012.

[148] *CFD Vision 2030 Study: A Path to Revolutionary Computational Aerosciences*. NASA, 2014.

[149] The three codesign centers are the Exascale Co-design Center for Materials in Extreme Environments (ExMatEx), the Center for Exascale Simulation of Advanced Reactors (CESAR), and the Center for Exascale Simulation of Combustion in Turbulence (ExaCT). Each center is a collaboration among DOE national laboratories, academic institutions, and, in the case of CESAR, private sector partners. The scope of work at each center is designed to have broad impacts across the energy technology landscape. More information on codesign and the three centers is available at http://science.energy.gov/ascr/research/scidac/co-design/.

[150] Proposals for future colliders, such as the international linear collider (ILC) and compact linear collider (CLIC), will collide electrons and positrons at hundreds of GeV in separate linear accelerators. The ILC would be based on SRF technology. The CLIC accelerators utilize a drive beam acceleration approach that enables very high accelerating gradients (up to 100 MV/m). More information is available at http://www.linearcollider.org/.

[151] The proposed high luminosity upgrade to the Large Hadron Collider will increase luminosity or the number of proton-proton collisions by an order of magnitude. The upgrade depends on technology developments in superconducting magnets, very compact and precise superconducting RF cavities, and high-power superconducting links. More can be found at http://hilumilhc.web.cern.ch.

[152] At the energy frontier, researchers accelerate particles to the highest energies ever achieved by humanity and collide them to produce and study the fundamental constituents of matter and the architecture of the universe. At the intensity frontier, researchers use a combination of intense particle beams and highly sensitive detectors to make extremely precise measurements of particle properties, study some of the rarest particle interactions predicted by the standard model of particle physics, and search for new physics. For more information see https://science.energy.gov/hep/research.

[153] Nuclear physics research activities in the low, medium, and high energy regime all depend on advanced accelerator technology. For example, the relativistic heavy ion collider (RHIC) is a 2.4 mile ring accelerator capable of colliding beams of heavy ions up to uranium. The Argonne Tandem LINAC Accelerator System (ATLAS) is a superconducting linear accelerator enabling study of nuclear structure and nuclear astrophysics for elements from hydrogen to uranium. More information about these and other facilities and about the nuclear physics program generally is available at http://www.science.energy.gov/np.

[154] The seven grand challenges for accelerator research are described in more detail in the 2012 Accelerator Task Force report available at http://www.acceleratorsamerica.org/report/accelerator_task_force_report.pdf.

[155] SRF cavities are resonators capable of achieving extraordinarily high (1,010) quality factors, providing very low energy loss and narrow bandwidth. This means that nearly all of the electrical energy can be applied to accelerating the beam and thus reducing the number of accelerating elements necessary to achieve a specified energy. SRF cavities are an enabling technology for future accelerators and upgrading existing accelerator facilities. More information can be found at http://www.fnal.gov or in Padamsee, H. S. "Superconducting Radio-Frequency Cavities." *Annual Review of Nuclear and Particle Science* (64), 2014; pp. 175-196. Available at: http://www.annualreviews.org/doi/abs/10.1146/annurev-nucl-102313-025612.

[156] Upgrades to the relativistic heavy ion collider completed in 2012 increased luminosity by approximately four times and was enabled in part by a new 56 MHz SRF system and installation of 3D stochastic cooling. See Fischer, W. (May 2010) "RHIC Luminosity Upgrade Program." The 1st International Particle Accelerator Conference, 23 May-28 May, 2010. Upton, NY: Brookhaven National Laboratory, pp. 1227-12312010. Accessed August 21, 2015: http://accelconf.web.cern.ch/AccelConf/IPAC10/papers/tuxmh01.pdf.

[157] The 12 GeV upgrade to CEBAF is enabled by installation of 10 new superconducting RF accelerating elements and upgrades to the magnets in the recirculation arcs to increase their strength. More information is available at https://www.jlab.org/12-gev-upgrade.

[158] Fermilab and TJNAF will jointly be building the next generation SRF cavities and associated cryomodules that will enable development of the 4 GeV superconducting LINAC at the heart of the LCLS-II upgrade. More information is available at http://www-bd.fnal.gov/LCLS.

[159] For more information about ASTA, see http://www.fnal.gov/pub/science/particle-accelerators/asta.html. For more information about TEDF, see https://www.jlab.org/.

[160] Plasma wakefield acceleration relies on density waves in a plasma to transfer energy from a "drive" beam to an "accelerated" beam, much like a surfer can be accelerated by ocean waves. Because material ionization limits do not apply to plasmas, accelerating gradients well in excess of 50 GeV/m have been demonstrated.

[161] The laser system at BELLA is capable of producing 40 joule pulses 40 femtoseconds in duration at one hertz frequency. More information is available at http://loasis.lbl.gov/.

[162] Plasma wakefield acceleration R&D is also conducted at the Argonne Wakefield Accelerator Facility (AWAF) at ANL. AWAF maintains the world's two highest charge RF photoinjectors capable of 100 nC per bunch. More information is available at http://gate.hep.anl.gov/awa/.

[163] The 2013 Workshop on Laser Technology for Accelerators explores the R&D needed to bridge the gap between current laser systems and those needed for future accelerators. The workshop report is available at http://science.energy.gov/~/media/hep/pdf/accelerator-rd-stewardship/Lasers_for_Accelerators_Report_Final.pdf.

[164] Available at: http://www.bnl.gov/atf/.

[165] For more information on the development of compact light sources, see the 2010 "Report of the Basic Energy Sciences Workshop on Compact Light Sources." Available at: http://science.energy.gov/~/media/bes/pdf/reports/files/CLS.pdf.

[166] "Accelerators for America's Future." Washington, DC: U.S. Department of Energy, 2010. p. 6. Available at: http://science.energy.gov/~/media/hep/pdf/accelerator-rd-stewardship/Report.pdf.

[167] For an example of increased solar cell efficiency due to transition metal doping, see Kranz, L.; Gretener, C.; Perrenoud, J.; Schmitt, R.; Pianezzi, F.; La Mattina, F.; Blösch, P.; Cheah, E.; Chirilă, A.; Fella, C.M.; Hagendorfer, H.; Jäger, T.; Nishiwaki, S.; Uhl, A.R.; Buecheler, S.; Tiwari, A. N. "Doping of Polycrystalline CdTe for High-efficiency Solar Cells on Flexible Metal Foil." *Nature Communications* (4), 2013. Available at: http://www.nature.com/ncomms/2013/130813/ncomms3306/full/ncomms3306.html. For a review of heteroatom doping in carbon-based materials for energy applications, see Paraknowitsch, J. P.; Thomas, A. "Doping Carbons Beyond Nitrogen: An Overview of Advanced Heteroatom Doped Carbons with Boron, Sulphur and Phosphorus for Energy Applications." *Energy & Environmental Science* (6:10), 2013; pp. 2839-2855. Available at: http://pubs.rsc.org/en/content/articlelanding/2013/ee/c3ee41444b#!divAbstract.

[168] For example, replacement of thermal techniques for drying metal coatings, which currently use approximately 166 MW of power, with electron beam technology could realize energy reductions of 95%. More examples of energy savings enabled by accelerator technology are described in "Accelerators for America's Future." Available at: http://science.energy.gov/~/media/hep/pdf/accelerator-rd-stewardship/Report.pdf.

[169] For example, a pilot facility in Poland uses electron beams to turn a mixture of flue gas and ammonia into saleable fertilizer. A pilot facility for electron beam treatment of waste water is currently operating in Korea. See "Accelerators for America's Future," available at http://science.energy.gov/~/media/hep/pdf/accelerator-rd-stewardship/Report.pdf, for additional examples.

[170] In close consultation with other Office of Science programs, the Office of High Energy Physics maintains an accelerator stewardship program to support accelerator R&D for applications outside discovery science. The myriad ways in which electron and ion accelerators are impacting society are described in the 2012 report "Accelerators for America's Future," available at http://science.energy.gov/~/media/hep/pdf/accelerator-rd-stewardship/Report.pdf and at the associated Web site http://www.acceleratorsamerica.org/index.html.

[171] Leemans, W. P.; Gonsalves, A. J.; Mao, H.-S.; Nakamura, K.; Benedetti, C.; Schroeder, C. B.; Tóth, C.; Daniels, J.; Mittelberger, D. E.; Bulanov, S. S.; Vay, J.-L.; Geddes, C. G. R.; Esarey, E. "Multi-GeV Electron Beams from Capillary-Discharge-Guided Subpetawatt Laser Pulses in the Self-Trapping Regime." *Physical Review Letters* (113:24), 2014; pp. 245002-1–245002-5. Available at: http://dx.doi.org/10.1103/PhysRevLett.113.245002.

[172] Demarteau, M.; Yurkewicz, K. "Tools, Techniques, and Technology Connections of Particle Physics." U.S. Department of Energy, Office of Science, May 2014. Available at: http://science.energy.gov/~/media/hep/pdf/files/Banner%20PDFs/TTT-connections-May14.pdf.

[173] Ibid.

[174] "Neutron and X-ray Detectors." Report of the Basic Energy Sciences Workshop on Neutron and X-ray Detectors. Washington, DC: U.S. Department of Energy Office of Science Office of Basic Energy Sciences, 2012. Available at: http://science.energy.gov/~/media/bes/pdf/reports/files/NXD_rpt_print.pdf.

[175] The full list of priority research directions are high-efficiency hard X-ray sensors, replacement of He-3 in neutron detectors, fast-framing X-ray detectors, high-speed spectroscopic X-ray detectors, very high-energy-resolution X-ray detectors, low-background signals, high-spatial resolution neutron detectors, improved acquisition and visualization tools, and improved analysis work flows.

[176] The production responsibility for certain isotopes does not reside within IDPRA. This includes commercially available isotopes, the medical isotope molybdenum-99, isotopes for reactor fuels (uranium), and isotopes for weapons (e.g., plutonium and tritium).

[177] The IPF facility (https://www.lanl.gov/science-innovation/science-programs/office-of-science-programs/nuclear-physics/isotopes/index.php) provides radioisotopes for a variety of applications, including medical diagnostics, fundamental nuclear physics, national security, environmental science, and industrial applications. Selected isotopes, including aluminum-26 and silicon-32, are only produced at IPF. IPF utilizes a 100 MeV proton beam extracted from the main Los Alamos Neutron Science Center and directed to a modern target irradiation facility.

[178] The BLIP facility (www.bnl.gov/cad/Isotope_Distribution/Isodistoff.asp) prepares commercially unavailable radioisotopes for applications in nuclear medicine and other industries as well as R&D for production of new radioisotopes of interest to nuclear medicine. BLIP uses 200 MeV protons from the BNL LINAC, which is primarily used as an injector for the Relativistic Heavy Ion Collider.

[179] Hot cell capabilities managed by the IDPRA are located at ORNL, LANL, PNNL, and BNL.

[180] The DOE Isotope Program supports the extraction of He-3 from the NNSA tritium reserves and distributes it throughout the federal complex according to federal allocation processes. The DOE Isotope Program leads a White House Interagency group that determines and coordinates the He-3 distribution for federal purposes and was responsible for successfully mitigating the He-3 shortage from 2008.

[181] The Isotope Program distributes a modest inventory of lithium-7 from the NNSA Y-12 facility for researchers and for manufacturing of radiation dosimeters. The nuclear power sector, which uses lithium-7 for modifying the chemistry in reactor cooling water systems, is currently reliant on Russian exports to meet demand. The Isotope Program is also currently supporting research on new methods of lithium-7 enrichment.

[182] As of 2015, the DOE Isotope Program has supported the development of radioisotope production capabilities or isotope production R&D at seven universities: University of Washington; University of California-Davis; University of Wisconsin; University of Missouri; Washington University; Texas A&M University; and Duke University. Available at: https://isotopes.gov/sites/sites.html.

[183] Available at: https://isotopes.gov.

[184] Gamma-ray photons emitted by positron-emitting radionuclides are used in positron emission tomography to produce 3D images of the body. Many of the isotopes used, including carbon-11, nitrogen-13, and oxygen-15, have sufficiently short half-lives that on-site preparation via small cyclotrons is required. Production of radioisotopes or isotope pairs with both therapeutic and diagnostic/imaging capabilities (theranostics) is a growing area isotope production research.

[185] Alpha particles produced by alpha decay are helium nuclei with an overall charge of 2+ and energy of approximately 5 MeV. They are highly ionizing and interact strongly with matter but have low penetrating power.

[186] The Isotope Program supports the only domestic source of californium-252 production.

[187] Multiple stable isotopes that are only available from Russia or the Netherlands are precursors to radioactive isotopes having applications in medicine, security, and manufacturing, among others. For example, strontium-88 is the precursor to strontium-89, which is used to treat bone cancer. Nickel-62 is the precursor to radioactive nickel-63, which is used as the active radiation source in detection systems for explosives and drugs. Selenium-74 is the precursor to selenium-75, which is used as a gamma radiography source.

[188] A burning plasma is one in which the fusion process itself provides the dominant heat source for sustaining the plasma temperature.

[189] ITER, located in Cadarache facility, Saint-Paul-lès-Durance, France, is designed to produce 500 MW of power while requiring only 50 MW to operate.

[190] The upgrade to NSTX doubled the magnetic fields strength and plasma current and increased plasma pulse length from one to five seconds.

[191] DIII-D and NSTX-U have different aspect ratios, defined as the ratio of the plasma radius dimension to the major radius of the confinement device. Aspect ratio is a leading factor imbedded in the physical laws governing stability of a fusion plasma confined in a toroidal geometry.

[192] A current list of the SC-FES SciDAC partnerships is provided in Supplemental Information (section 9B).

[193] The science challenges and applications of low temperature (or partially ionized) plasmas were articulated during the 2008 Fusion Energy Sciences Workshop on Low Temperature Plasmas. The resulting report, "Low Temperature Plasma Science: Not Only the Fourth State of Matter but All of Them," is available at http://science.energy.gov/~/media/fes/pdf/workshop-reports/Low_temp_plasma_workshop_report_sept_08.pdf.

[194] (a) Paz-Soldan, C.; Nazikian, R.; Haskey, S. R.; Logan, N. C.; Strait, E. J.; Ferraro, N. M.; Hanson, J. M.; King, J. D.; Lanctot, M. J.; Moyer, R. A.; Okabayashi, M.; Park, J-K.; Shafer, M. W.; Tobias, B. J. “Observation of a Multimode Plasma Response and Its Relationship to Density Pumpout and Edge-Localized Suppression.” *Physical Review Letters* (114:10), 2015; pp. 105001-1-5 . Available at: http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.114.105001#fulltext. (b) Nazikian, R.; Paz-Soldan, C.; Callen, J. D.; deGrassie, J. S.; Eldon, D.; Evans, T. E.; Ferraro, N. M.; Grierson, B. A.; Groebner, R. J.; Haskey, S. R.; Hegna, C. C.; King, J. D.; Logan, N. C.; McKee, G. R.; Moyer, R. A.; Okabayashi, M.; Orlov, D. M.; Osborne, T. H.; Park, J-K.; Rhodes, T. L.; Shafer, M. W.; Snyder, P. B.; Solomon, W. M.; Strait, E. J.; Wade, M. R. “Pedestal Bifurcation and Resonant Field Penetration at the Threshold of Edge-Localized Mode Suppression in the DIII-D Tokamak.” *Physical Review Letters* (114:10), 2015; pp. 105002-1-5 . Available at: http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.114.105002.

[195] “Computational Materials Science and Chemistry: Accelerating Discovery and Innovation Through Simulation-Based Engineering and Science.” Report of the Department of Energy Workshop on Computational Materials Science and Chemistry for Innovation, July 26–27, 2010. Available at: http://science.energy.gov/~/media/bes/pdf/reports/files/cmsc_rpt.pdf.

[196] “From Quanta to the Continuum: Opportunities for Mesoscale Science.” A Report for the Basic Energy Sciences Advisory Committee Mesoscale Science Subcommittee, September, 2012. Available at: http://science.energy.gov/~/media/bes/pdf/reports/files/OFMS_rpt.pdf.