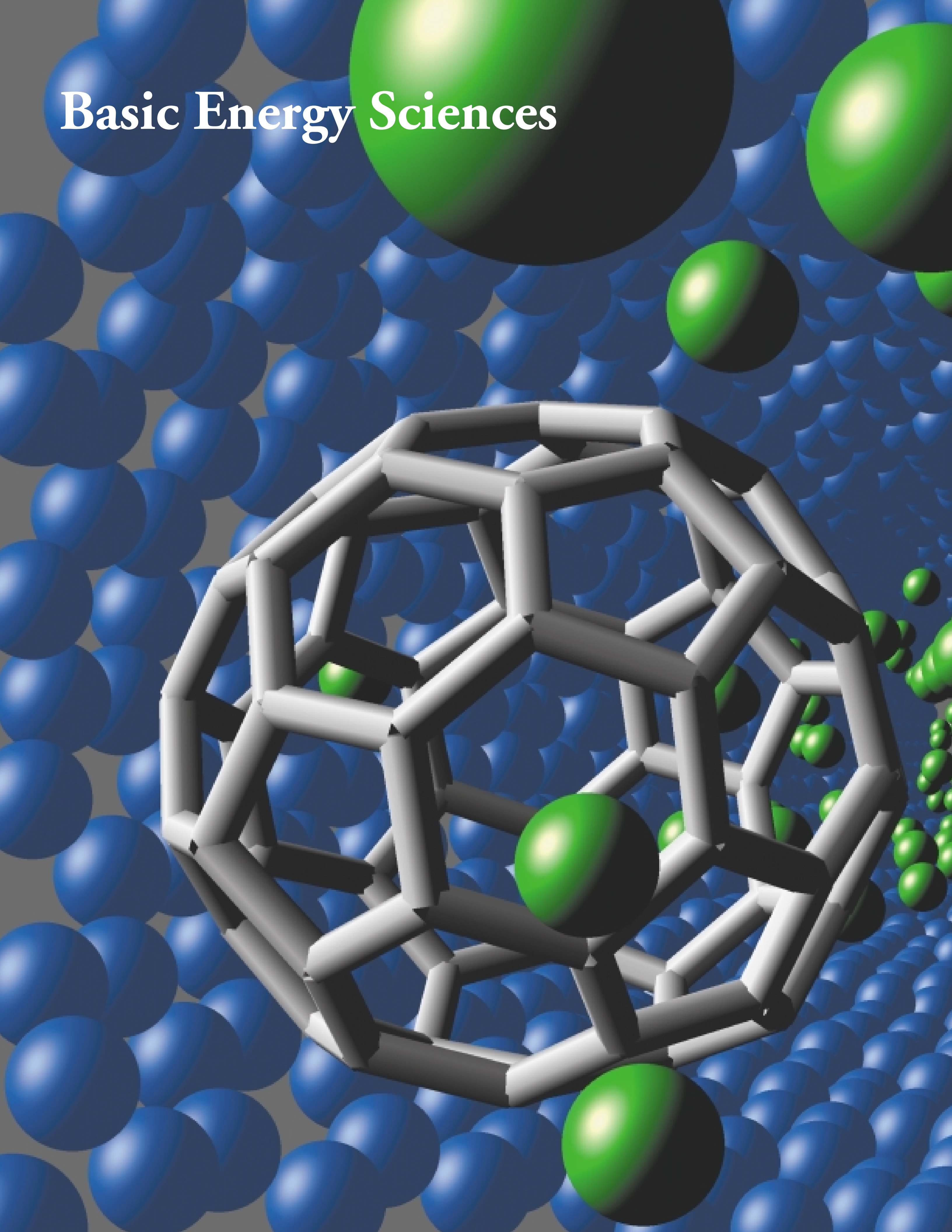
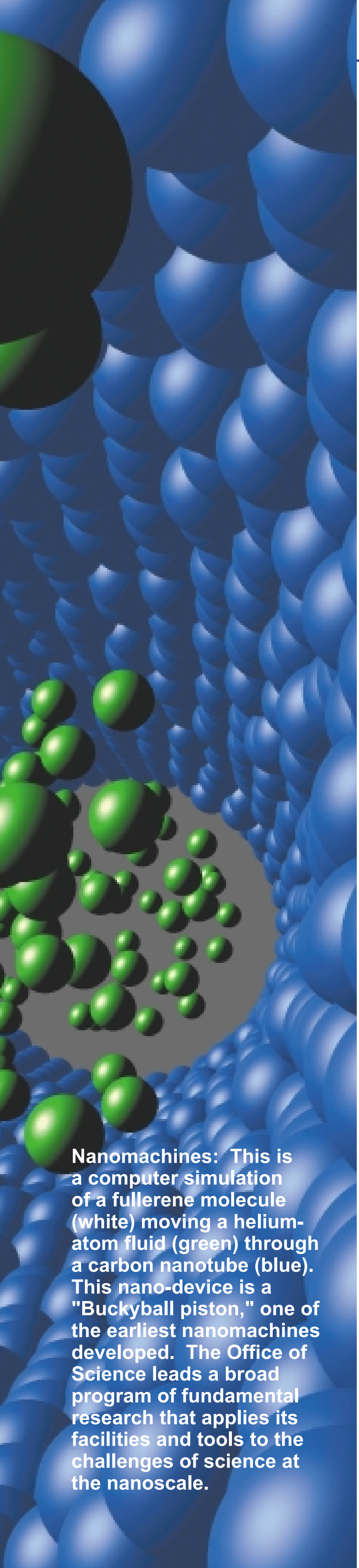
Basic Energy Sciences





Nanomachines: This is a computer simulation of a fullerene molecule (white) moving a helium-atom fluid (green) through a carbon nanotube (blue). This nano-device is a "Buckyball piston," one of the earliest nanomachines developed. The Office of Science leads a broad program of fundamental research that applies its facilities and tools to the challenges of science at the nanoscale.

LBNL

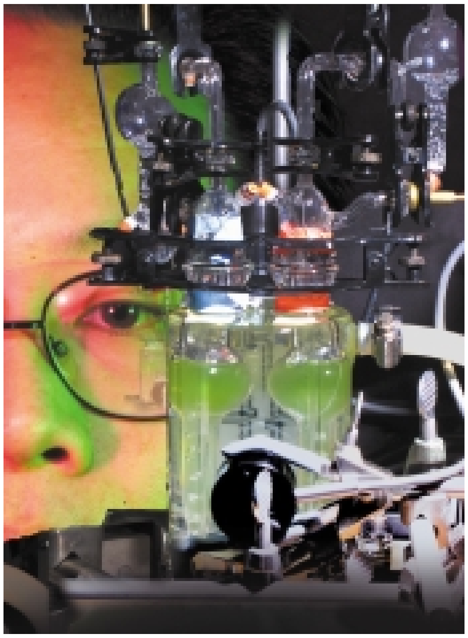
1

Advance the Basic Sciences for Energy Independence

Provide the scientific knowledge and tools to achieve energy independence, securing U.S. leadership and essential breakthroughs in basic energy sciences.

The growth of our economy over the past half-century has derived in substantial part from steady improvements in our energy technologies. In each subsequent decade, we have produced more goods and services with a given amount of energy, and we have produced that energy more efficiently and with less environmental impact. Much of this progress has come from advances in the materials and chemical sciences such as new magnetic materials; high strength, lightweight alloys and composites; novel electronic materials; and new catalysts, with a host of energy technology applications. We are now in the early stages of two remarkable explorations—observing and manipulating matter at the molecular scale and understanding the behavior of large assemblies of interacting components. Scientific discoveries in these two frontiers alone will accelerate our progress toward more efficient, affordable, and cleaner energy technologies. They pose some of the most fascinating and far-reaching scientific challenges of our time:

- What new, useful properties do materials display as we move from the classical or macroscopic world to objects composed of a few to a few thousands of atoms or molecules?
- What range of optical, mechanical, catalytic, electrical, tribological, and other properties can be achieved by designing devices and materials at the molecular scale?
- How can we efficiently assemble molecular-scale structures? How do living organisms construct complex assemblies, and can we apply these approaches to engineer useful devices and materials?
- How can we control chemical reactivity—the making and breaking of chemical bonds—to produce energy and desired materials while eliminating unwanted byproducts?



ORNL

Hydrogen from microalgae: Hydrogen may be one of the best resources to fuel the future economy of America and the world. It can be produced not only with resources such as petroleum, coal, and natural gas, but also from plants and organic waste. DOE's Office of Science, working in partnership with the Office of Energy Efficiency, has unlocked the secret to increasing the hydrogen yield of a certain type of green microalgae that shows promise of producing hydrogen cheaply, easily, and cleanly. This research is a collaboration among the National Renewable Energy Laboratory, Oak Ridge National Laboratory, and the University of California at Berkeley.

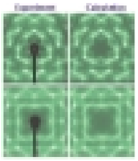
- How can we design, model and exploit complex systems—systems composed of large numbers of interacting components and/or components operating at different spatial or temporal scales—such as novel magnetic or superconducting materials?

Our ability to answer these and related questions depends on our ability to observe, characterize, manipulate, and computationally model matter at the atomic or molecular scale. This is a fundamentally interdisciplinary effort, linking science and engineering, and providing the foundation for a broad spectrum of scientific and technical advances. Essential tools for this research include current generation synchrotron x-ray and neutron scattering sources, and the more advanced sources to come, higher resolution electron microscopes and other atomic probes, and terascale computers. The Office of Science will deliver the leading-edge tools, sustain the interdisciplinary research, and create the knowledge necessary to realize the extraordinary potential of the basic energy sciences to meet our energy and other critical needs.

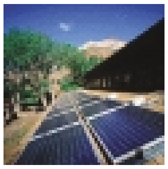
As an integral part of this Strategic Plan, and in *Facilities for the Future of Science: A Twenty-Year Outlook*, we have identified the need for eight future facilities to realize our Basic Energy Sciences vision and to meet the science challenges described in the following pages. Two of the facilities are near-term priorities: the **Linac Coherent Light Source (LCLS)** and the **Transmission Electron Achromatic Microscope (TEAM)**. The LCLS will provide laser-like radiation 10 billion times greater in power and brightness than any existing x-ray light source, enabling the study of matter and chemical reactions at speeds and levels of detail well beyond what is currently possible. TEAM will be the first of a new generation of electron microscopes that, by correcting for distortions in focus inherent to all current electron microscopes, will give much clearer images and allow the use of much larger experimental chambers. All

Our History of Discovery…Select Examples

1960-1994
Revealed the enzymatic mechanism of the molecule adenosine triphosphate (ATP), the energy currency of living cells.
(1997 Nobel Prize)

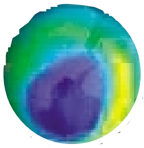


1980s
Developed synchrotron radiation light sources, which made many science discoveries possible such as ultra-high density computer hard drives.



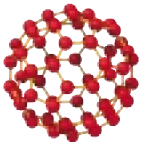
1980-2000
Achieved materials breakthroughs that reduced the cost of solar electricity by 100-fold.

1960 *1970* *1980*



1974
Discovered the effect of CFCs on the ozone layer, providing the scientific knowledge to protect our living planet.
(1995 Nobel Prize)

1981
Developed new opto-electronic materials and devices for wireless communications, semiconductor lasers, supermarket scanners, remote sensing, and medical diagnostics.



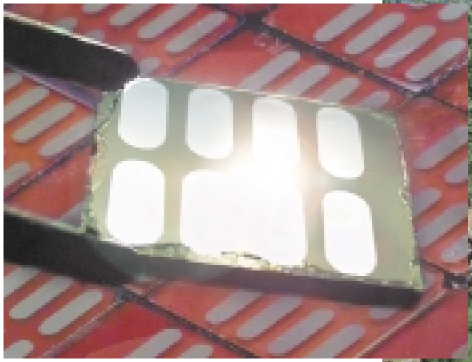
1985
Discovered a new class of carbon structure—the Buckyball.
(1996 Nobel Prize)

eight facilities are included in our Basic Energy Sciences Strategic Timeline at the end of this chapter and in the facilities chart in Chapter 7 (page 91), and they are discussed in detail in the *Twenty-Year Outlook*.

Our Strategies

1.1 Advance the core disciplines of the basic energy sciences, producing transformational breakthroughs in materials sciences, chemistry, geosciences, energy biosciences, and engineering.

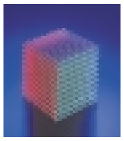
The Office of Science will advance leading-edge research programs in the natural sciences, emphasizing fundamental research in materials sciences, chemistry, geosciences, and aspects of biosciences encompassed by the DOE missions, and it will provide world-class, peer-reviewed research results that are responsive to our Nation's energy security needs as well as the needs of the broad scientific community. As part of a thorough program of fundamental research, the Office of Science will implement a comprehensive plan based on the findings and recommendations of the Basic Energy Sciences Advisory Committee workshop, *Basic Research Needs to Assure a Secure Energy Future*. For example, new materials will be developed that impact solid-state lighting, smart windows, vehicular transportation, thermoelectric conversion, hydrogen storage, electrical storage, and improved fuel cells, leading to significant increases in efficiency. In addition, new catalysts will be designed that exert exquisite control over chemical reactions so as to specify the reaction products and the rates at which they form.

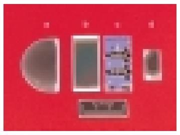

LBNL


NREL

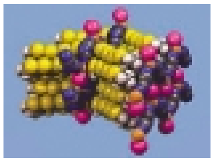
Nanoscience for energy applications: The photovoltaic array on the south roof of the Visitor Center at Zion National Park provides a significant portion of the electricity needs for the building as well as an uninterrupted power supply for use during power outages. DOE's Office of Science, working in partnership with the Office of Energy Efficiency, has provided the research that has improved solar cell efficiency and reduced solar energy costs 100-fold. New nanoscience research is bringing chemists, materials scientists, physicists, and theorists together to create devices such as this hybrid solar cell (offset left), which combines nanotechnology with plastic electronics. The result is a photovoltaic device that is cheaper and easier to manufacture than current semiconductor counterparts.

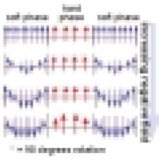

1986
Discovered organic-based magnets that are lighter, more flexible, and less energy-intensive to make than conventional magnets.

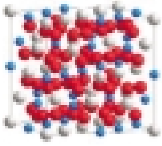

1990
Developed photonic bandgap crystals for revolutionary control of light propagation for sensors, antennas, lasers, solar cells, and telecommunications equipment.


1996
Developed lithium batteries with high-energy storage capacity and virtually no adverse environmental impact.

1990 *2000*


1990
Developed the first purely organic superconductors.


1993
Advanced the science of magnetic materials and paved the way for the manufacture of magnet structures with greater mechanical strength and stability.


1998
Discovered material to immobilize plutonium—gadolinium zirconate.

"The biggest single challenge for the next few decades: Energy for 10 billion people! At minimum we need 10 terawatts of power from some clean new energy source by 2050. For worldwide peace and prosperity, we need it to be cheap."

—Richard Smalley, shared the 1996 Nobel Prize in Chemistry for the discovery of fullerenes (Buckyballs)

The ability to simulate accurately the behavior of a system under many different conditions can enhance the effectiveness of experimental investigation and can even replace experiments in cases where they are too difficult or too expensive. There are a large number of areas of research in the natural sciences where simulation could have an enormous impact. Our ability to simulate has lagged behind what we can see experimentally, mostly due to major bottlenecks in the application of theory and computation in modeling the behavior of single atoms and molecules within a larger, more complex system.

Advanced crystallization processes: Scientists pursuing better and cheaper crystals for laser fusion have developed a "rapid-growth" method for producing the world's largest single crystal optical elements—crystals that weigh 600 to 700 pounds. By understanding and controlling the crystallization process at the molecular level, complex microstructures can be synthesized that will affect disciplines and technologies ranging from pharmaceuticals (such as crystallized proteins, among them human insulin) to new optical materials. This rapid-growth method was developed by DOE's Office of Science in partnership with the National Nuclear Security Administration to supply the crystal plates for the giant laser in the National Ignition Facility (NIF), which is currently under construction at Lawrence Livermore National Laboratory. This large-scale rapid-growth crystal growing technique is expected to save millions of dollars for both construction and later operation of the NIF, which will also help to maintain the safety and reliability of the Nation's nuclear weapons stockpile.

LLNL

To help realize this strategy, the synchrotron radiation light sources, electron-beam microcharacterization centers, and neutron scattering facilities will help reveal the atomic details of metals and alloys; glasses and ceramics; semiconductors and superconductors; polymers and biomaterials; proteins and enzymes; catalysts, sieves, and filters; and materials under extremes of temperature, pressure, strain, and stress. Using these powerful probes of science, we will be able to design new materials, atom-by-atom, and observe their creation as they unfold. Once the province of specialists, mostly physicists, these facilities are now used by thousands of researchers annually from all disciplines.

Our strategy includes the following emphases:

- Using the foundation of programs in materials sciences, chemistry, geosciences, energy biosciences, and engineering, create new options for the production, storage, distribution, and conservation of energy with basic research in areas such as hydrogen, nano-designed materials, nuclear fuel cycles and actinide chemistry, heterogeneous catalysis, novel membrane assemblies, and innovative energy conversion pathways.
- Remove simulation bottlenecks in order to accelerate the pace of scientific discovery, for example, bridge electronic-through-macroscopic length and time scales; simulate opto-magneto-electronic properties of materials;

understand chemical reactivity in solutions, solids, and turbulent flows; and explore a systems approach to molecular recognition, self-assembly, and chemical reactivity.

- Complete construction of the Spallation Neutron Source, which will be the world's most intense pulsed neutron source, and which will enable the study of materials that were previously not accessible to study. It is scheduled for commissioning in 2006.
- Design and construct the revolutionary x-ray light source called the LCLS to provide laser-like radiation in the x-ray region of the spectrum that is 10 billion times greater in peak power and peak brightness than any existing source. The high brilliance of the ultra-short pulses from the LCLS might make it possible to obtain the structure of a single molecule using only one pulse of light, a vast improvement over current methods.
- Explore new concepts in electron microscopy that will allow previously unimaginable studies of materials structure, chemistry, and the effect of external forces on materials during deposition, reaction, and deformation at the subnanometer level.

ORNL

Spallation Neutron Source (SNS): This accelerator-based neutron source facility will provide the most intense pulsed neutron beams in the world for scientific research and industrial development. Neutron research helps scientists and engineers improve materials used in high-temperature superconductors; powerful lightweight magnets; aluminum bridge decks; and stronger, lighter plastic products. The SNS is currently being built at Oak Ridge National Laboratory in collaboration with Argonne National Laboratory, Brookhaven National Laboratory, Lawrence Berkeley National Laboratory, Los Alamos National Laboratory, and Thomas Jefferson National Accelerator Facility, and will be completed in 2006.

1.2 Lead the nanoscale science revolution, delivering the foundations and discoveries for a future built around controlled chemical processes and materials designed one atom at a time or through self-assembly.

The main elements of the Office of Science nanoscale research program are the establishment of five Nanoscale Science Research Centers (NSRCs) and the support for nanoscale research in targeted areas addressing forefront science and DOE mission needs. The NSRCs are a new way of doing business for the dispersed cottage industry of researchers currently working on the enormous set of problems that together define "nanoscale science." The ability to fabricate complex structures using chemical, biological, and other synthesis techniques; characterize them; assemble them; integrate them into devices; and do all this in one place will change the way materials research is done. Our strategy includes the following emphases:

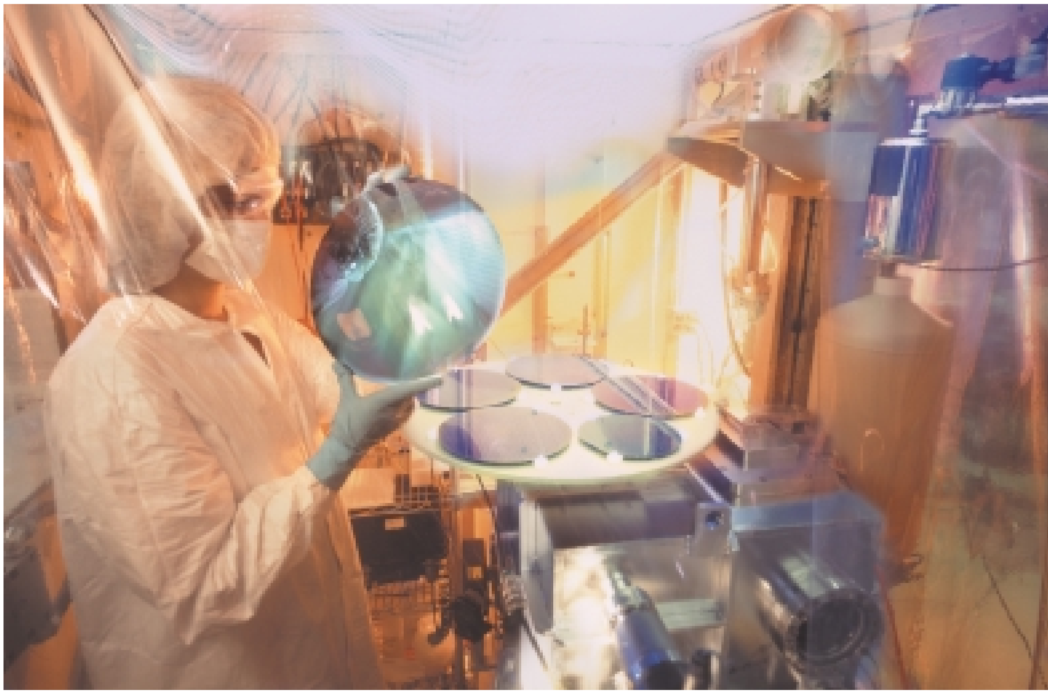
- Attain a fundamental understanding of phenomena unique to the nanoscale.

Nanoscale Science Research Centers: The Office of Science will build five new Nanoscale Science Research Centers to provide the Nation's research community with world-class resources for the synthesis, processing, fabrication, and analysis of materials at the nanoscale. User programs being initiated at the Centers will give the research community immediate access to their emerging capabilities.

- Achieve the ability to design and synthesize materials at the nanoscale to produce materials with desired properties and functions, using as necessary the tricks and tools of Nature's assemblies, both living and nonliving.
- Integrate nanoscale objects into microscale assemblies and macroscale devices.
- Develop experimental characterization tools and theory/modeling/simulation tools to advance nanoscale science.

1.3 Master the control of energy-relevant complex systems that exhibit collective, cooperative, and/or adaptive behaviors, i.e., systems that cannot be described as the sum of their parts.

Entering this century, we find science and technology at yet another threshold: the study of simplicity will give way to the study of "complexity" as the unifying theme. The triumphs of science in the past century, which improved our lives immeasurably, can be described as elegant solutions to problems reduced to their ultimate simplicity. The new millennium is taking us into the world of complexity. Here, simple structures interact to create new phenomena, assembling themselves into devices that begin to answer questions that were, until the 21st Century, the stuff of science fiction. Understanding collective, cooperative, and adaptive phenomena and emergent behavior takes many forms. Our strategy includes the following emphases:


SLAC

Stanford Synchrotron Radiation Laboratory: Physicists build particle accelerators to explore the fundamental nature of matter. However, bending the particle beams produces synchrotron radiation. First viewed as a problem, this radiation was soon recognized as an ultrapowerful beam—a pinpoint of light 30 times brighter than the sun. Scientists use it to study a wide range of materials at the Stanford Linear Accelerator Center (SLAC) (as depicted above) and at other Office of Science light sources around the U.S. Now, an important tool of science, synchrotron radiation produces leading-edge discoveries spanning many fields and disciplines within the materials and life sciences.

- Understand interactions among individual components that lead to coherent behavior that often can be described only at higher levels than those of the individual units. This can produce remarkably complex and yet organized behavior.
- Explore electrons interacting with each other and with the host lattice in solids that can give rise to magnetism and superconductivity.
- Investigate chemical constituents interacting in solution that can give rise to complex pattern formation and growth.
- Research and learn to synthesize and adapt the processes that underlie living systems, whereby they self-assemble their own components, self-repair as necessary, and reproduce; explore how they sense and respond to even subtle changes in their environments.

Our Timeline and Indicators of Success

Our commitment to the future, and to the realization of **Goal 1: Advance the Basic Sciences for Energy Independence**, is not only reflected in our strategies, but also in our Key Indicators of Success, below, and our Strategic Timeline for Basic Energy Sciences (BES), at the end of this chapter.

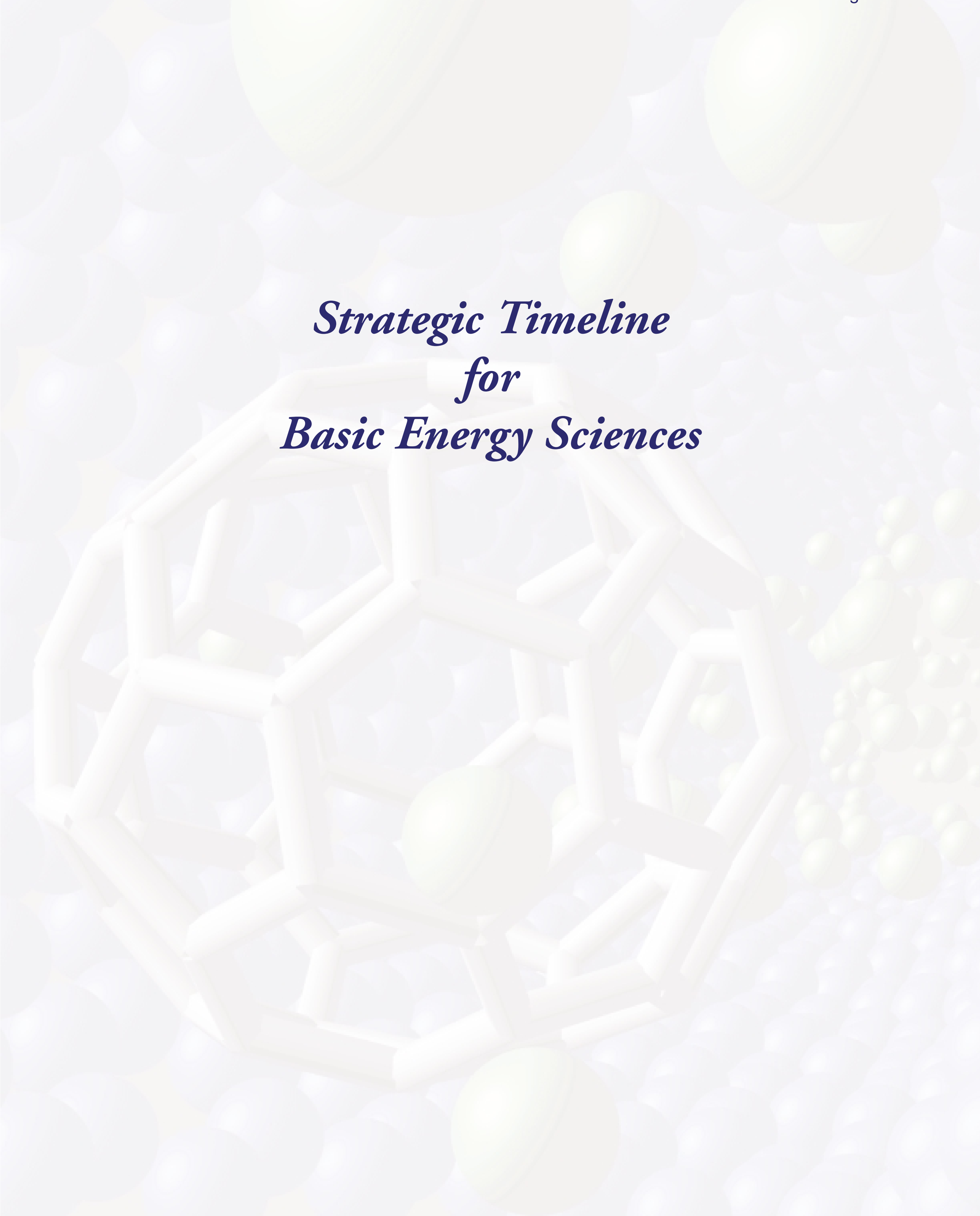
Our BES Strategic Timeline charts a collection of important, illustrative milestones, representing planned progress within each strategy. These milestones, while subject to the rapid pace of change and uncertainties that belie all science programs, reflect our latest perspectives on the future—what we hope to accomplish and when we hope to accomplish it—over the next 20 years and beyond. Following the science milestones, toward the bottom of the timeline, we have identified the required major new facilities. These facilities, described in greater detail in the DOE Office of Science companion report, *Facilities for the Future of Science: A Twenty-Year Outlook*, reflect time-sequencing that is based on the general priority of the facility, as well as critical-path relationships to research and corresponding science milestones.

Additionally, the Office of Science has identified Key Indicators of Success, designed to gauge our overall progress toward achieving Goal 1. These select indicators, identified below, are representative long-term measures against which progress can be evaluated over time. The specific features and parameters of these indicators, as well as definitions of success, can be found on the web at **www.science.doe.gov/measures.**

Key Indicators of Success:

- Progress in designing, modeling, fabricating, characterizing, analyzing, assembling, and using a variety of new materials and structures, including metals, alloys, ceramics, polymers, biomaterials, and more—particularly at the nanoscale—for energy-related applications.
- Progress in understanding, modeling, and controlling chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic, organic, self-assembling, and biological systems.
- Progress in developing new concepts and improving existing methods for solar energy conversion and other major energy research needs identified in the Basic Energy Sciences Advisory Committee workshop report, *Basic Research Needs to Assure a Secure Energy Future.*
- Progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Strategic Timeline for Basic Energy Sciences



Strategic Timeline—E

2003 2005 2007 2009 2011 2013

The Science

Core Disciplines of the Basic Energy Sciences

- Establish a program to develop computational tools for simulation, virtual testing, and design of materials (2006)

- Increase hydrogen production through chemical, biochemical, and biomimetic systems (2011)
- Realize improvements in hydrogen and fuel cells through modest earlier investments in basic research (2011)

- Initiate research programs on hydrogen production and storage methods (2005)
- Initiate research programs on materials degradation in hostile environments (2005)
- Initiate expansion of materials, chemistry, and biochem programs (2005)
- Complete joint strategic plan and roadmap with the Office of Nuclear Energy (2005)

- Complete first draft GEN IV material properties database in support of nuclear power (2010)

- Test biofilms for ability to generate electricity from organic waste (2007)
- Identify key physical processes that help maintain stability of materials during neutron irradiation (2007)

Nanoscale Science

- Enable the production of new composite materials and joining technologies with fabrication at the nanoscale (2011)

Energy-Relevant Complex Systems

- Develop new tools and advanced computers to enable scientists to simulate and model materials of much greater complexity for new energy technologies (2007)

- Design various complex interactions of atomic and molecular species to exhibit new physical phenomena for use in new energy applications (2011)

Future Facilities**

Linac Coherent Light Source (LCLS): The LCLS will provide laser-like radiation 10 billion times greater in power and brightness than any existing x-ray light source.

Transmission Electron Achromatic Microscope (TEAM): TEAM will be the first of a new generation of electron microscopes.

Spallation Neutron Source (SNS) 2-4 MW Upgrade: The SNS upgrade will more than double its power.

SNS Second Target Station: The second target station at the SNS will provide a long wavelength neutron source.

***These strategic milestones are illustrative and depend on funds made available through the Federal budget process.**

****For more detail on these facilities and the overall prioritization process, see the companion document, *Facilities for the Future of Science: A Twenty-Year Outlook.***

Basic Energy Sciences*

2015 2017 2019 2021 2023 2025

- Enable hydrogen and other low-carbon fuels to become significant components of the U.S. energy portfolio due to the accomplishment of one or more BES grand challenges (2025)

- Develop new materials that enable the widespread use of solid state lighting, improved fuel cells, breakthroughs for materials in radiation environments, new battery concepts, advanced membranes, hybrid solar cells, smart materials, and more (2015)
- Enable the practical start of the hydrogen economy with new knowledge on hydrogen production, storage, and use (2015)

- Enable the efficient, inexpensive conversion of sunlight to products such as fuels (2025)

- Use the complexity of matter as an asset rather than an obstacle by "tuning" the properties of matter with small changes in composition or with the application of pressure or a magnetic field (2025)

National Synchrotron Light Source Upgrade (NSLS II): The NSLS upgrade will create and install the next-generation design for a synchrotron light source storage ring.

Advanced Light Source (ALS) Upgrade: The ALS upgrade will allow the facility to expand to accommodate new instruments to explore the traditionally difficult spectral region at the border between optics and electronics (called the "terahertz-gap").

Advanced Photon Source (APS) Upgrade: The APS upgrade will create a "super storage ring" of electrons that will greatly enhance the brilliance of the facility.

High-Flux Isotope Reactor (HFIR) Second Cold Source and Guide Hall: Construction of the cold source and guide hall at HFIR will complete the facility, more than doubling its capabilities.