Seeing Matter at Atomic and Molecular Scales

From Nanoscale Structure to Macroscale Properties

Studying matter at the level of atoms and molecules requires measuring structures that are **billionths of a meter (nanometers)** or less in size. This nanoscale realm is where the fundamental properties of materials are established. Melting temperature, magnetic properties, charge capacity, and even color are dictated by the arrangements of atoms and molecules. The ability to understand, design, and control these properties will lead to a new world of materials and technologies for numerous application areas.

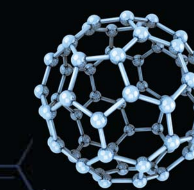
An atom's typical size is tenths of a nanometer. The wavelength range of visible light is a few hundred nanometers, which is too large to detect atoms. **Seeing matter at the level of atoms requires instruments that can measure structures that are one thousand times smaller than those detectable by the most advanced light microscopes.** Thus, to characterize structures with atomic detail, we must use probes such as **x-rays, electrons, and neutrons** that are at least as small as the atoms being investigated.

The fundamental tenet of materials research is that **structure determines function**. Advanced tools based on x-ray, electron, and neutron beams are providing atomic details of metal alloys, plastics, enzymes, superconductors, carbon nanostructures, and materials under extremes of temperature, pressure, and stress. **Models and simulations** empowered by supercomputers are helping researchers test theories and explore the nanoscale dynamics of materials with greater realism (see central figure). By advancing our **atom-by-atom understanding** of material structure, we open up a dazzling array of possibilities for **designing new materials with desired properties and functions**.

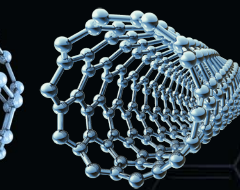
How do only 118 building blocks—all the known elements in the periodic table—combine to create every substance on Earth? How do these atoms make materials with a seemingly endless variety of forms and properties—soft and hard, ductile and brittle, magnetic and nonmagnetic, insulating and superconducting, living and nonliving? Why do the same atoms connected in varying ways yield remarkably different materials? Finding out is key to creating the materials and technologies needed to thrive in an age of natural resource, environmental, and fiscal constraints. This quest begins with visualizing atoms (nuclei and electrons) and their interactions.

Carbon: The Many Faces of the Sixth Element

Seemingly minor changes in the positions and connections among atoms can yield materials with very different physical properties. For example, carbon atoms can assemble into diverse structural forms—diamond, graphite and graphene, carbon nanotubes, and fullerenes (buckyballs)—each with unique characteristics. By tapping nature's secrets for building matter atom by atom, nanotechnology researchers can design and build a new generation of nanostructures that outperform existing materials.

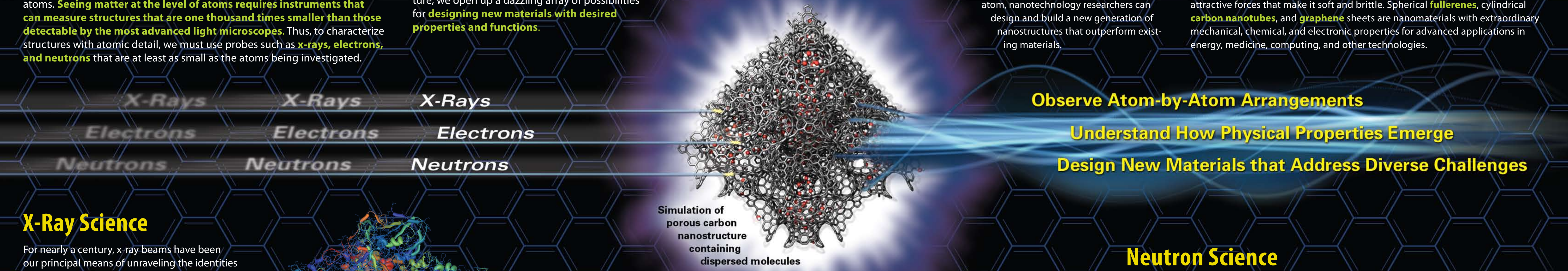


Fullerene (C_{60})



Carbon nanotube

In **diamond**, each carbon atom forms strong covalent bonds with four other carbon atoms, making it the hardest natural substance known. In **graphite**, many one-atom-thick layers of carbon are held together by weak attractive forces that make it soft and brittle. Spherical **fullerenes**, cylindrical **carbon nanotubes**, and **graphene** sheets are nanomaterials with extraordinary mechanical, chemical, and electronic properties for advanced applications in energy, medicine, computing, and other technologies.



Simulation of porous carbon nanostructure containing dispersed molecules

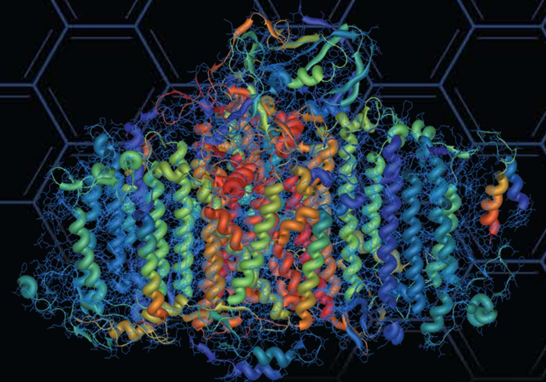
Observe Atom-by-Atom Arrangements

Understand How Physical Properties Emerge

Design New Materials that Address Diverse Challenges

X-Ray Science

For nearly a century, x-ray beams have been our principal means of unraveling the identities and positions of atoms in crystallized samples ranging from relatively simple metal materials to highly complex biological molecules like proteins and DNA. Due to their short wavelength, hard x-rays are very useful for probing atomic structure. Today's synchrotron radiation and free-electron laser light sources produce x-rays so intense that they have vastly eclipsed historical methods and have given rise to scores of new ways to do experiments.

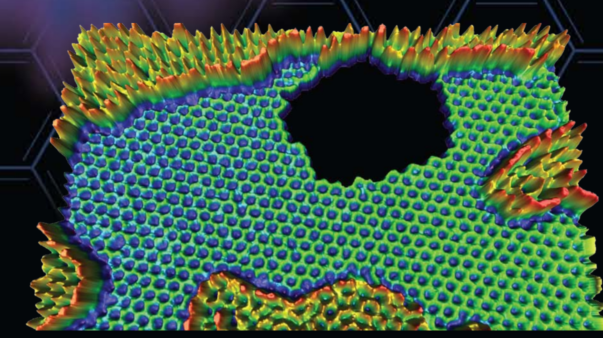


Photosystem I is a complex, membrane-bound molecular machine in plant cells that converts sunlight to energy during photosynthesis. Membrane proteins represent an important class of macromolecules targeted by industrial biotech companies and drug developers.

Crystallized samples of materials are analyzed by passing x-rays through them. The x-rays are scattered by the atoms of a crystal, producing a diffraction image on detectors. This image provides unique information on the identity of the atoms and structure of the crystal. Large, flexible membrane proteins, such as Photosystem I in plant cells, form very small crystals that tend to be imperfect and weakly diffracting. Intense x-ray sources have been invaluable for determining the structures and properties of such macromolecules.

Electron Science

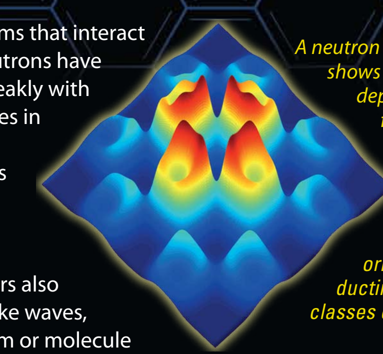
Because of the strong interactions between negatively charged electrons and the charged particles in matter, electron beams can provide important structural and chemical information underlying the behavior of various materials. Today's most advanced electron microscopes can produce electron beams that are so bright they can be used to visualize subnanometer phenomena such as the electronic structure and bonding of atoms. By understanding the atom-by-atom assembly of materials into stable configurations, researchers are gaining new insights into improving existing materials and synthesizing new nanostructures with superior strength, durability, corrosion resistance, and other desired properties.



Powerful electron microscopy provides real-time imaging of atoms repositioning themselves along the edge of a hole blown through a sheet of graphene, a one-atom-thick layer of carbon atoms. Understanding stable edge arrangements may hasten development of advanced electronic devices based on carbon's outstanding electronic and structural properties. The raised features are adsorbed molecules.

Neutron Science

Unlike x-rays and electron beams that interact with a material's electrons, neutrons have no charge and thus interact weakly with the electrically charged particles in materials. As a result, neutrons serve as nondestructive probes that can scatter directly off atomic nuclei deep within a material. Neutron beams from research reactors or accelerators also can act like magnets, diffract like waves, and set particles within an atom or molecule into motion. Analyzing the neutrons that scatter off the sample reveals structural and magnetic information. Scientists worldwide use neutrons to study the arrangement, motion, and interaction of atoms in materials. As an important complement to x-ray diffraction and electron microscopy, neutron-based research provides valuable information that is not obtainable from other techniques.



A neutron scattering spectrum shows time- and space-dependent magnetic fluctuations in a superconductor. The observed fourfold symmetry of the spin excitations suggests a common origin for superconducting states in different classes of materials.

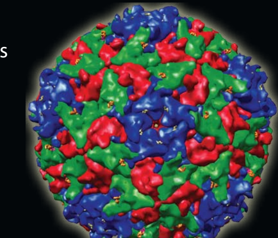
Atomic-Scale Insights Drive Discovery and Innovation for Real-World Solutions

More Durable Building Materials

Cement is a widely used building material, but little is known about the nanoscale properties of this "glue" that holds concrete structures together. X-ray scattering studies have confirmed a highly ordered arrangement of 3.5-nanometer crystals within calcium silicate hydrate, the most important binding agent in cement. With more detailed structural information, stronger cement formulations could be created, potentially saving hundreds of millions of dollars in infrastructure maintenance and repair costs.

Potential Anticancer Agent

Using an x-ray beamline, the 3-D structure has been solved for Seneca Valley Virus-001, a virus that attacks certain cancer cells without harming normal human cells. This virus exhibits a cancer-killing specificity 10,000 times higher than traditional chemotherapeutics in animal studies. By investigating how the virus uses its bumpy patchwork coat of proteins to interact with cancer cell receptors, drug designers hope to develop anticancer viruses for many different types of cancer cells.



High-Temperature Superconductors

About 10% of all electricity generated today is lost to resistance during transmission. Superconductors are materials that conduct electricity without resistance, but conventional types require ultralow temperatures (near absolute zero). Neutron scattering studies of superconductors are providing key insights into how magnetic properties and atomic arrangements influence superconductivity at higher temperatures. Unraveling the mechanisms for achieving high-temperature superconductivity could lead to much more efficient systems for producing, delivering, and using electricity.

Next-Generation Energy Storage

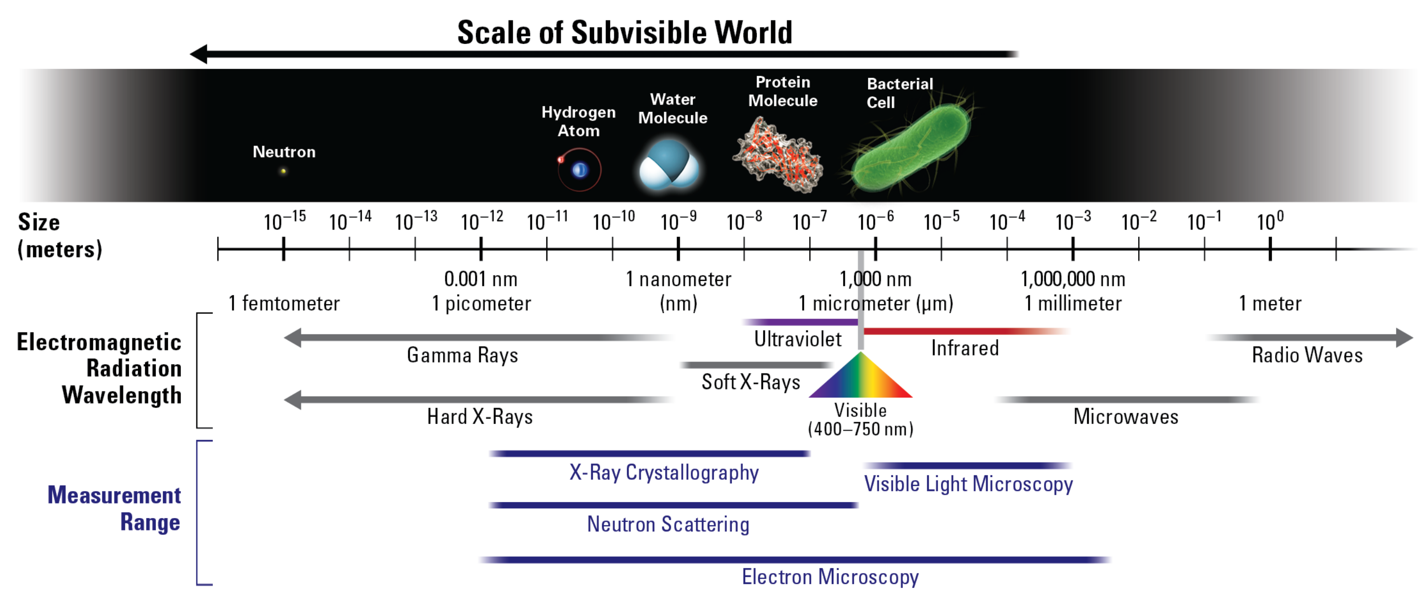
Our technology-driven society demands improvements in batteries that power cell phones, laptops, and electric cars and advances in systems that reliably store and deliver electricity from solar, wind, and other sources. New microscopy and neutron scattering techniques are tracking the flow of ions through energy storage materials and revealing the degradation that results from charging and discharging. Understanding these nanoscale processes will inform the design of next-generation devices that can store more energy, charge faster, and last for thousands of charge-discharge cycles.

User Facilities: Tools for Seeing Atoms

Revealing the atomic-scale secrets of materials requires a variety of cutting-edge imaging and analytical instruments that use beams of different types of particles or radiation. These beams of x-rays, neutrons, and electrons provide complementary information about various aspects of a material's nanoscale structure. These techniques together are revealing insights that enable us to understand and ultimately control the properties of materials.

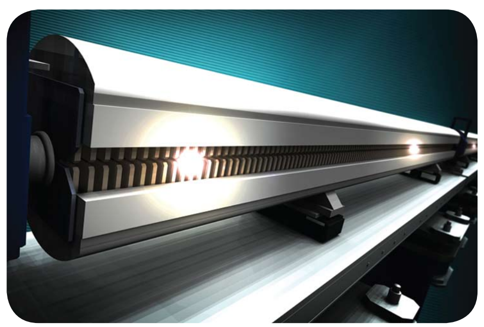
Building on investments made by the Department of Energy (DOE) and its predecessor agencies in pioneering work to develop nuclear reactors and particle accelerators, the DOE Office of Science today provides the research community with a suite of scientific user facilities—x-ray light sources, neutron sources, and electron-beam microcharacterization centers—to explore the atomic world. Since their inception in the 1970s, the growth of scientific user facilities worldwide has been remarkable. Major scientific user facilities make possible experimental studies that cannot be done in ordinary laboratories, and these facilities have created a new style of research in which scientists conduct investigations that benefit from a merging of ideas and techniques from different disciplines.

Together, these DOE facilities help more than 10,000 researchers pursue discoveries that improve the economy, energy options, medical treatments, technologies, and our fundamental understanding of the materials that make up our world. The leading-edge research conducted at these facilities has earned numerous awards, including Nobel prizes in chemistry, physics, and medicine. Selected facilities are described below.



X-Ray Light Sources

Millions of times brighter than medical x-rays, light sources generate high-quality, stable beams of x-rays and other electromagnetic radiation that can be used for numerous experimental techniques. Electrons are deflected as they travel past bending magnets along the circular track of a synchrotron or through other specially designed magnetic devices. This creates a continuous spectrum of radiation with various wavelengths and strengths (e.g., ultraviolet light and hard or soft x-rays) that scientists can select to suit their particular experiment. These rays are then sent down pipes called beamlines to sophisticated instruments in work areas or end stations where studies are conducted.



Each 2-m-long, 1-ton undulator at LCLS contains many "teeth," or alternating pairs of north-south magnets that force electrons to follow a wavy path, creating x-rays.

The **Advanced Photon Source (APS)** is the largest scientific user facility in the United States (its electron storage ring could encircle a major-league baseball stadium). By bending accelerated electrons into a circular path with magnetic fields, the APS produces ultrabright radiation in the hard x-ray range that can be focused onto small samples, allowing researchers to quickly gather large amounts of detailed data. With over 60 beamlines equipped with numerous instruments customized to particular research needs, the APS offers a broad range of experimental capabilities.

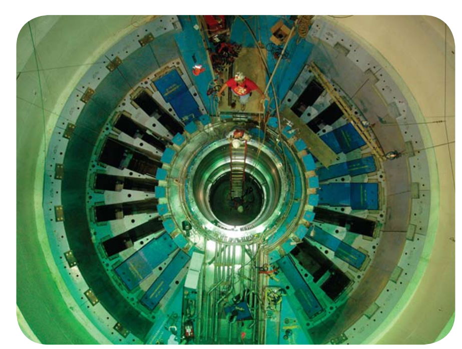
The **Linac Coherent Light Source (LCLS)** is an x-ray free-electron laser that is used much like a super high-speed strobe flash that produces very short pulses of electrons. The LCLS electron beam is linear, and the electrons travel through a 1-kilometer-long accelerator before emitting x-rays as they slalom back and forth within the final 100-meter stretch of undulators. The waves of x-rays become synchronized as they further interact with the electron pulses. The resulting ultrafast pulses of hard x-rays allow scientists to take stop-motion pictures of moving molecules, shedding light on the fundamental processes of chemistry, technology, and life itself.

Neutron Sources

Neutrons are produced for scientific experiments in a reactor or using an accelerator-based process called spallation. By bombarding a heavy-element target (e.g., mercury) with accelerated protons, spallation causes some neutrons to be knocked out or "boiled off" as the bombarded nuclei heat up. When the energetic protons collide with the heavy atomic nuclei in the target, about 20 to 30 neutrons are expelled from each nucleus.

Neutrons from these sources are guided through beamlines to the sample material being investigated. The neutrons bounce off the sample, scattering in different directions. Where they bounce, how fast, and where they land reveal details about the sample's properties. Special detectors measure these scattering patterns and send the data to a computer for various analyses and processing, which often include reconstructing a three-dimensional image of a sample's nanoscale architecture. Such images provide unique insights into a material's structure, dynamics, and magnetic properties.

The **Spallation Neutron Source (SNS)** is a pulsed accelerator-based neutron source. Before hitting a target, protons are accelerated to very high energies and passed into a ring where they accumulate in bunches. Each bunch is released from the ring as a pulse, creating a neutron beam 10 times more intense than any other such source in the world. Each pulse contains neutrons in a range of wavelengths and energies tuned to a specific experiment by moderators. The highest energy neutrons are moderated to room temperature or cooler. Cooling neutrons slows their speed and lengthens their wavelengths to levels suitable for analyzing certain magnetic properties or studying the larger structural components of "soft" materials such as proteins and polymers.



The SNS chamber contains the central liquid mercury target that is bombarded by protons to produce spallation neutrons.

Electron-Beam Microcharacterization

More than a thousand times smaller than neutrons, electrons are tiny, negatively charged particles that can be energized, deflected, or focused into beams by electric and magnetic fields. Electrons interact so strongly with the nuclei and electrons of atoms that they scatter with much higher intensity than x-rays or neutrons, thereby generating powerful signals from small numbers of atoms and even from just a single atom. These attributes make electrons very useful not only for characterizing matter at subnanometer to micrometer scales but also for capturing images of individual atoms within a sample.

TEAM is the world's most powerful electron microscope.

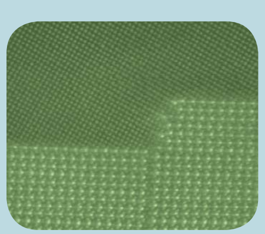
The **National Center for Electron Microscopy (NCEM)** at Lawrence Berkeley National Laboratory is home to the Transmission Electron Aberration-corrected Microscope (TEAM). TEAM is the product of a collaboration among DOE electron-beam experts to develop the first electron microscope to surpass a spatial resolution of 0.05 nanometers, roughly half the diameter of a hydrogen atom.

An electron gun atop the TEAM instrument applies an intense electrical field and heat to emit electrons from a source material. The electron gun accelerates and focuses the emitted electrons into a tight beam traveling at more than half the speed of light. The accelerated electrons behave like waves with very short wavelengths. Once shot from the electron gun, the beam is condensed and directed toward the sample. The electron waves zoom through the sample and into a series of magnetic lenses that magnify and focus them to form an image on a screen at the bottom of the microscope column. As they pass through the magnetic lenses, some electron waves are bent at different angles, blurring the image. TEAM components correct these aberrations, giving this instrument its unprecedented capability of directly imaging subatomic distances with ultrahigh precision.

Measurement Techniques for Instruments Using X-Ray, Electron, and Neutron Beams

Imaging

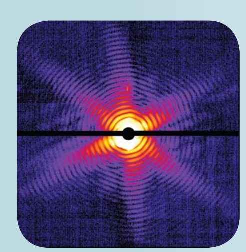
Imaging techniques use particle beams to obtain pictures with fine spatial resolution of materials. Microscopy using electrons or x-rays is now powerful enough to image individual atoms within a structure, reveal local physical properties by measuring small shifts in the positions of atoms, and study molecular events that last only one millionth of a billionth of a second.



Arrangement of atoms in an aluminum alloy.

Scattering

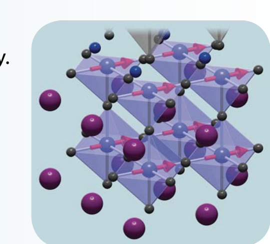
Scattering or diffraction occurs when a stream of particles or a wave strikes an object and is deflected from its original trajectory. When a particle beam is aimed at a sample, some of these particles will interact with nuclei or with the electrons surrounding nuclei and bounce away at an angle. The scattering pattern created when the "bounced" particles hit a detector gives information about the structure of the sample.



X-ray diffraction of a single virus particle.

Spectroscopy

Spectroscopy is the study of the interactions between matter and radiated energy. The spectrum of wavelengths or frequencies of energies absorbed or emitted by the sample under investigation contains information about the electronic structure of the matter, such as the nature of its chemical bonds or the behavior of its electrons during excitation.



Electron orbital positioning of a metal oxide interface revealed by x-ray spectroscopy.

Scientific User Facilities

U.S. Department of Energy, Office of Science
Office of Basic Energy Sciences

X-Ray Light Sources

National Synchrotron Light Source (NSLS)
Brookhaven National Laboratory, Upton, New York

Stanford Synchrotron Radiation Lightsource (SSRL)
SLAC National Accelerator Laboratory, Menlo Park, California

Advanced Light Source (ALS)
Lawrence Berkeley National Laboratory, Berkeley, California

Advanced Photon Source (APS)
Argonne National Laboratory, Argonne, Illinois

Linac Coherent Light Source (LCLS)
SLAC National Accelerator Laboratory, Menlo Park, California

Aerial view of the Advanced Photon Source

Neutron Scattering Facilities

Spallation Neutron Source (SNS)
Oak Ridge National Laboratory, Oak Ridge, Tennessee

High Flux Isotope Reactor (HFIR)
Oak Ridge National Laboratory, Oak Ridge, Tennessee

Manuel Lujan Jr. Neutron Scattering Center (Lujan Center)
Los Alamos National Laboratory, Los Alamos, New Mexico

Aerial view of the Spallation Neutron Source

Electron-Beam Microcharacterization Centers

Electron Microscopy Center (EMC)
Argonne National Laboratory, Argonne, Illinois

National Center for Electron Microscopy (NCEM)
Lawrence Berkeley National Laboratory, Berkeley, California

Shared Research Equipment (SHaRE) User Facility
Oak Ridge National Laboratory, Oak Ridge, Tennessee

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