Purpose
To study catalysts and enzymes for basic and applied research in chemistry, biology, materials science, and energy conservation.

Sponsor
U.S. Department of Energy: Office of Basic Energy Sciences, Office of Fossil Energy, Office of Transportation Technologies, and Chemical & Biological Non-Proliferation Program; National Institutes of Health; U.S. Army Medical Research Institute of Infectious Diseases

BNL departments participating
Biology, Chemistry, Energy Sciences & Technology, Materials Sciences, and Physics

BNL research racilities
- *National Synchrotron Light Source*
- *Scanning Transmission Electron Microscope*

Research techniques
cluster deposition, extended x-ray absorption fine structure spectroscopy (EXAFS), in situ time-resolved x-ray powder diffraction, laser ablation, low-temperature microcrystallography, molecular beam scattering, near-edge x-ray absorption fine structure spectroscopy (NEXAFS), photoemission, reflection absorption infrared spectroscopy (RAIRS), scanning tunneling microscopy (STM), surface x-ray scattering (SXS), structure-based drug design, x-ray crystallography, x-ray diffraction, and x-ray scattering

Collaborating institutions
U.S.: *Argonne National Laboratory, Johns Hopkins University, Lawrence Livermore National Laboratory, Louisiana State University, Mayo Clinic Cancer Center, Oak Ridge National Laboratory, Rutgers University, Sandia National Laboratory, State University of New York at Buffalo, State University of New York at Stony Brook, University of Delaware, University of Michigan, University of South Carolina, University of South Florida, University of Utah, University of Wisconsin-Milwaukee, Yale University*
international: *Karolinska Institute, Sweden; Universidad Central de Venezuela; University of Aarhus, Denmark; University of Bergen, Norway; University of Paris V, France; University of Saragosa, Spain; Venezuelan Institute of Scientific Research*

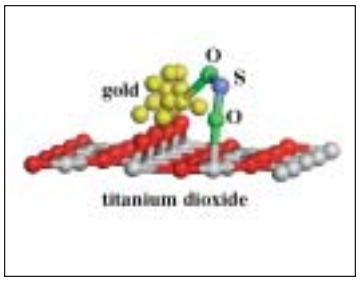
Industrial partners
Accelrys, Chevron Texaco, Dow Chemical, Miravant Medical Technologies, 3M Corporation

Web address
http://nslsweb.nsls.bnl.gov/nsls/Default.htm

Understanding Catalysts and Enzymes

Using synchrotron light to probe atomic motion

The National Synchrotron Light Source (NSLS) at Brookhaven Lab produces beams of very intense x-rays, ultraviolet, and infrared light. These beams allow scientists to investigate the structure and properties of many materials, including catalysts and enzymes.



The decomposition of sulfur dioxide (SO_2) by a catalyst made of gold nanoparticles over titanium dioxide, a process used to remove sulfur from gasoline.

Acting like chemical "matchmakers," catalysts and enzymes help bring reactants together, resulting in faster chemical and biological reactions. The catalyst or enzyme participates but is not consumed in the reaction.

Understanding catalysts and enzymes could lead to greater control over chemical reactions and advances in areas as diverse as chemistry, biology, materials science, and energy conservation.

Catalysis studies at Brookhaven:

- Structural studies that reveal, over time, the changes undergone by catalysts while they bring the reactants together.
- Investigations of more efficient fuel cells. Fuel cells are environmentally friendly sources of energy that may one day replace thermal combustion engines.
- The design and production of nanocatalysts, which are made of small arrays or clusters of 100 to 10,000 atoms deposited on metal and metal oxide surfaces. Nanocatalysts can be used to improve the efficiency of catalytic converters, fuel cells, and chemical production.
- Investigations of the catalytic properties of crystal structures featuring stripe-shaped periodic patterns, obtained by depositing successive atomic layers on the surface of a bulk crystal. These structures can be used as nanocatalysts.
- The design of catalysts that could help reduce or eliminate sulfur compounds from gasoline and other fuels. Brookhaven scientists are pursuing two approaches called hydrodesulfurization and ultra-deep sulfur removal, based on bimetallics — compounds made of two metals — and nanocatalysts, respectively.
- Studies of zeolites, cavity-shaped crystals that can trap particles of specific sizes. Zeolites can be used as catalysts to transform carbon dioxide, a greenhouse gas, into methanol and methane, as well as to oxidize hydrocarbons.
- Studies of porphyrins, natural compounds present in photosynthesis and enzymes, to develop energy transducers, catalysts, chemical sensors, molecular wires, and photochemical cancer drugs.
- Studies of cytochrome b_5 reductase, the principal enzyme for normal functioning of hemoglobin, the protein that transports oxygen in the blood. Lack of this enzyme causes the disease methemoglobinemia, the symptoms of which include mental deficiency.
- Research into how enzymes called proteases degrade other proteins during housekeeping and regulatory functions of proteins in cells.
- Understanding the structure of the botulinum toxin, which may lead to the design of vaccines and drugs to prevent or treat botulism, a paralytic disease usually caused by the presence of the toxin in food.
- Use of structure-based drug design to develop new antiviral (adenovirus) and antibacterial (Chlamydia) agents with pathogen proteinases — protein-degrading enzymes — as targets.
- Research into how redesigned plant enzymes could be used to produce sources of materials and energy that are more environmentally friendly than fossil fuels.

Brookhaven National Laboratory is managed for the U.S. Department of Energy by Brookhaven Science Associates, a company founded by Stony Brook University and Battelle.

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