Science.

Technology.

Innovation.

Pacific Northwest National Laboratory

Institute for Interfacial Catalysis

The science of catalysis is not new. The word *catalysis* was coined by Swedish chemist Jöns Jakob Berzelius in the early 19th century to describe the modification of chemical reaction rates by substances (catalysts) that are unchanged when the reaction is complete. Today, industrial catalyst technologies affect nearly all areas of the chemical and petroleum industries, and the economic impact of catalysis has been estimated to be over 10 trillion dollars per year worldwide.

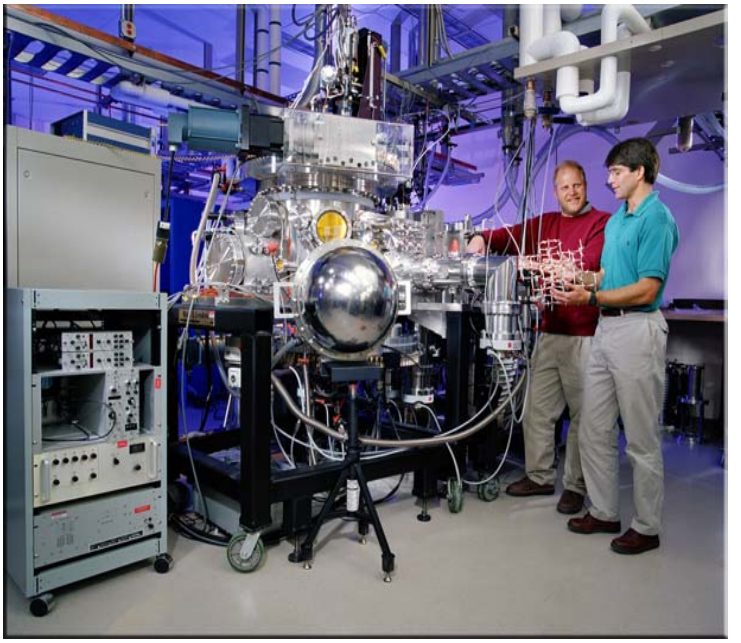
The grand challenge for catalysis science is to design catalyst structures to control catalytic activity and selectivity.

Our researchers are discovering new science that is underpinning the development of innovative catalyst materials and technologies to:

- **improve energy efficiency**
- **provide alternative energy and feedstock sources**
- **reduce environmental impacts from industrial processes.**

Diverse Catalysis Research and Development

Research at PNNL's Institute for Interfacial Catalysis (IIC) emphasizes a fundamental understanding of catalytic materials and the chemical reactions occurring on catalyst surfaces. We apply this understanding to developing industrial and environmental solutions such as catalyst materials and processes for efficient use of fossil fuels, development of advanced automobile catalytic converter devices, and production of value-added chemicals and fuels from bio-based feedstocks.



Advanced facilities for catalysis science are being used to provide a fundamental understanding of the catalytic materials and chemical reactions occurring on catalyst surfaces.

Institute for Interfacial Catalysis

Office of Science
U.S. DEPARTMENT OF ENERGY

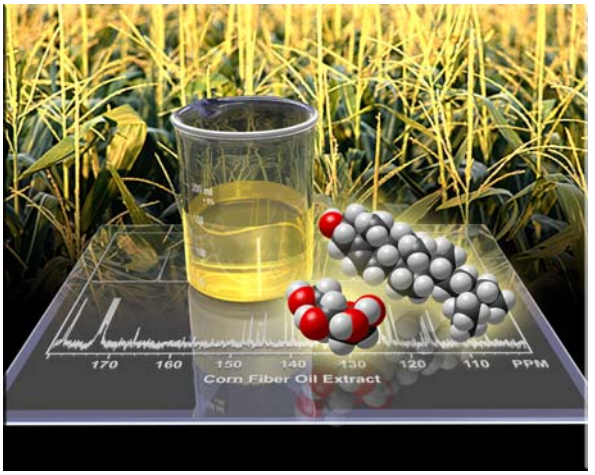
Pacific Northwest National Laboratory
Operated by Battelle for the U.S. Department of Energy

The addition of major new research capabilities, along with programs in the basic science aspects of catalysis, has further expanded our ability to provide new fundamental knowledge for the catalysis research community, and technical solutions for our clients.

Research Areas

Our research focus includes biomass conversion, environmental catalysis, solid oxide fuel cells, microchannel reactors for fuel and chemical production, and surface science studies of catalysts. Alongside these experimental efforts, computational chemistry is a core-competency that is becoming a world-leading resource for catalysis research and development.

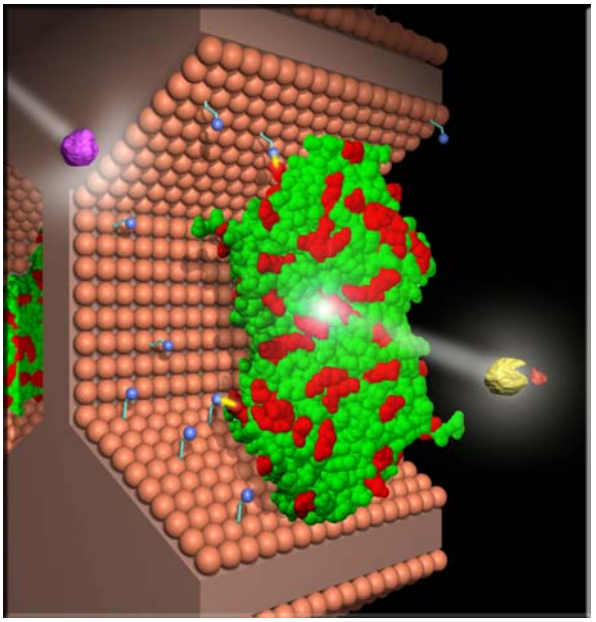
Fundamental Science: An important area of research involves furthering our fundamental understanding of the chemical reaction mechanisms that occur on catalyst surfaces, including identifying the catalytic sites directly involved in the rate-limiting elementary processes. The challenge is to develop precise control of chemical transformations using catalysis.



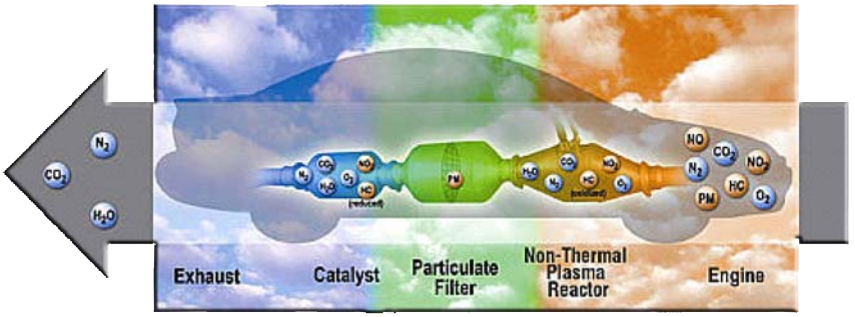
The most abundant core building blocks converted from corn fiber—glucose, xylose and arabinose—are being evaluated as a feedstock for either fermentation to ethanol or direct aqueous phase catalytic conversion to propylene glycol, ethylene glycol, and glycerol.

Biomass Conversion: Advancements in bio-products science and technology are resulting in new opportunities for grower associations, commodity processors, and chemical companies, as well as federal agencies interested in the environmental and economic benefits of renewable resources for production of high-value industrial and consumer products. Our research and development includes patented catalytic processes that convert sugars, acids, and fermentation-derived carbohydrates to high-value commodity and specialty chemicals.

Exhaust Emissions: IIC researchers are applying their internationally recognized expertise and capabilities in surface chemistry, catalyst mechanisms, computational modeling, material synthesis, and aerosols to address key challenges in diesel engine exhaust emissions abatement. Current research is focused on lean-NO_x traps, urea selective catalytic reduction, catalyzed



Biotechnology teams with nanotechnology for useful biocatalytic transformations: Specially developed enzymes (green) embedded in a synthetic catalyst support material, which was created to immobilize the enzymes and enhance their activity and stability, can perform useful chemical reactions (reactant, purple molecule at left; products, yellow to red molecules at right). Such nanostructures could eventually be used for a broad range of enzyme-based catalytic reactions to produce energy, remove or deactivate contaminants, and store carbon to mitigate global climate change.



Vehicle exhaust, loaded with nitric oxides, flows into the non-thermal plasma reactor, where it is converted into nitrogen dioxide. A catalyst then initiates chemical reactions that reduce nitrogen dioxide into harmless nitrogen gas.

The Milli-Watt System Fuel Processor, which includes a catalytic microreactor, converts methanol into hydrogen and carbon dioxide. The system contains the unit operations of a commercial-sized hydrogen plant—but approximately a billion times smaller in capacity and size.

soot filters, sulfur adsorbers, and a non-thermal plasma technology to enhance the hydrocarbon selective catalytic reduction of NO_x.

Microchannel Technology: Microtechnology greatly increases heat and mass transfer rates, resulting in highly efficient devices for chemical and thermal systems. These devices can be mass-produced using PNNL's patented "sheet architecture," which incorporates multiple microcomponents and unit operations within a laminated microstructure to produce very efficient, compact, and cost-effective systems. Highly active, long-life catalysts are engineered onto structured supports and integrated into the microchannels. These catalysts provide rapid heat and mass transfer rates while operating with a minimal pressure drop. New catalysts are being developed to take advantage of the unique chemical process environments afforded in these microreactor devices.

Solid Oxide Fuel Cells: Solid oxide fuel cells are being considered as one of the most attractive—efficient and clean—technologies for power generation, and catalysis plays an important role in their development. IIC researchers are conducting detailed studies of oxygen reduction kinetics at the cathode/electrolyte interface and fuel oxidation kinetics at the anode/electrolyte interface.

Our work includes gaining a better understanding of the catalysis, electrocatalysis, and surface electrochemistry under actual fuel cell operating conditions, as well as the influence of electrode composition, structure, preparation methods, etc. This information is being used to develop new catalytic anode and cathode materials.

Facilities

A wide range of leading-edge experimental and computational resources for catalysis research are located in the Environmental Molecular Sciences Laboratory (EMSL), a DOE national scientific user facility on the PNNL campus. These resources include EMSL's capabilities for ultra-high vacuum surface science, high-field nuclear magnetic resonance and electron spin resonance facilities, as well as high-speed computers and computational chemistry software, to address the fundamental aspects of the chemical reaction mechanisms that occur on catalyst surfaces. This is coupled with resources (facilities and expertise) unique in the DOE National Laboratory system to directly apply these basic research results to large and growing programs aimed at catalyst material and process development. These facilities include the Combinatorial Catalysis (CombiCat) Laboratory, a state-of-the-art integrated system for high-throughput catalyst experimentation, and the Exhaust Emissions Science Laboratory.

In the Exhaust Emissions Science Laboratory, researchers investigate methods for reducing engine emissions from current production vehicles and methods for more efficient future vehicles.

The William R. Wiley Environmental Molecular Sciences Laboratory is a national scientific user facility and research organization located at Pacific Northwest National Laboratory. EMSL, which is operated by PNNL for the U.S. Department of Energy's Office of Biological and Environmental Research, houses some of the world's most cutting-edge research equipment. More than 100 experimental systems are available for fundamental research at the molecular level. www.emsl.pnl.gov

Expertise

Our technical staff has broad catalyst expertise in a variety of disciplines, such as Physical Chemistry, Chemical Engineering, Inorganic Chemistry, Mechanical Engineering, Analytical Chemistry, Physics, Organic Chemistry, Materials Science, Radiation Chemistry, Chemical Physics, and Geochemistry.

More than 50 scientists and engineers obtain significant levels of DOE programmatic support for catalysis-related research. These staff include those widely recognized in the external community (e.g., ACS Awardees; Fellows of the American Vacuum Society); numerous staff whose thesis research and/or post-doctoral fellowships focused on catalysis; and, significantly, staff with considerable industrial experience in catalysis research at BP/Amoco, Catalytica, Cummins Engine Company, Dow, Engelhard, Exxon, and Union Carbide.

About PNNL

Pacific Northwest National Laboratory (www.pnl.gov), a U.S. Department of Energy Office of Science laboratory, solves complex problems in energy, national security, the environment, and life sciences by advancing the understanding of physics, chemistry, biology, and computation. PNNL employs more than 4000 staff, has a $650 million annual budget, and has been managed by Ohio-based Battelle since the lab's inception in 1965.

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