Pacific Northwest NATIONAL LABORATORY

Proudly Operated by **Battelle** *Since 1965*

Toward a secure energy future, our researchers are pursuing discovery science that is underpinning the development of innovative catalyst materials, processes, and technologies to:

- **Improve energy efficiency**
- **Provide alternative energy and feedstock sources**
- **Reduce environmental impacts associated with production, transport and utilization of energy.**

U.S. DEPARTMENT OF ENERGY

PACIFIC NORTHWEST NATIONAL LABORATORY

Institute for Interfacial Catalysis

Chemical transformations are at the heart of energy production and consumption, and catalysis lies at the core of efficient and effective use of our current energy sources, developing alternative energy sources, and reducing environmental impacts. Practiced for more than a century, fundamental research in catalysis is being newly invigorated by advances in capabilities to control, measure, and compute chemical and physical properties accurately and with exquisite spatial and temporal resolution.

The grand challenge for catalysis science in the 21st century is to understand how to design catalyst structures to control activity and selectivity, and then put this understanding to use in addressing a secure energy future for our nation.

The expertise and resources of the Institute for Interfacial Catalysis allow its researchers to perform discovery and applied science, while bridging these two, often separated, areas with science inspired by the end use.

DIVERSE CATALYSIS RESEARCH AND DEVELOPMENT

Research at Pacific Northwest National Laboratory's (PNNL's) Institute for Interfacial Catalysis takes a science-to-solutions approach. We provide 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 feedstock.

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.

SCIENTIFIC LEADERSHIP

A critical mass of more than 60 scientists and engineers in the Institute for Interfacial Catalysis contribute to catalyst-related research. Many of these staff are widely recognized in the external community. Our staff include American Chemical Society, American Vacuum Society, and North American Catalysis Society award winners.

The Institute for Interfacial Catalysis draws upon a broad range of disciplines to create synergistic, multidisciplinary teams that include experimental and theoretical chemistry, physics, chemical and mechanical engineering, materials

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

science, and computation. We also collaborate with recognized catalysis leaders at universities, international research institutes, and other national laboratories.

FACILITIES

The Institute for Interfacial Catalysis uses leading-edge experimental and computational resources, including

- Ultra-high vacuum surface and interface characterization
- High-field nuclear magnetic resonance spectroscopy
- Electron microscopy
- High-speed computers and computational chemistry software
- In-situ vibrational spectroscopy
- Wide array of catalytic reactors.

These resources are in the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL), a U.S. Department of Energy national scientific user facility. Additional resources exist in the Combinatorial Catalysis Laboratory (Combicat), a state-of-the-art integrated system for high-throughput catalyst experimentation; the Exhaust Emissions Science Laboratory; and other facilities in the national laboratory system.

▶ INNOVATIVE RESEARCH

Our approach synergistically combines computation and experimentation.

Fundamental Science: Answer grand challenges in catalysis science by determining reaction mechanism, and accounting for the behavior of materials on the basis of their structure at the atomic and molecular levels.

Theory, Modeling, and Simulations: Develop and apply complex quantum mechanical electronic structure and dynamical theories and methods to characterize and predict the fundamental processes that govern the chemical transformations of catalysis.

Computations: Run complex computer programs that embody the above theories and methods on powerful supercomputers for increasingly realistic models of catalytic systems and transformations.

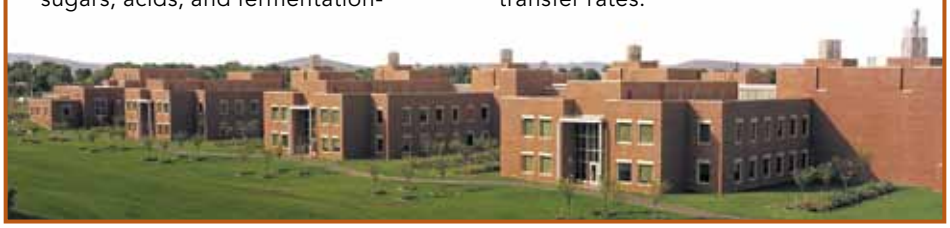
Biomass Conversion: Develop catalytic processes that convert sugars, acids, and fermentation-derived carbohydrates to high-value commodity and specialty chemicals.

Clean Coal: Develop improved catalysts and models for indirect and direct conversion of coal to liquid products, and technologies to minimize emission of toxic and greenhouse gases from coal gasification.

Exhaust Emissions: Answer scientific challenges to control emissions from fuel-efficient, "lean-burn" engines, such as diesels.

Alternative Energy: Provide predictive characterization of the factors controlling activity and selectivity in complex catalytic transformations relevant to the hydrogen economy and other new energy technologies.

Microchannel Technology: Design highly active, long-life catalysts to exploit the unique chemical process environments in microreactors that provide more rapid heat- and mass-transfer rates.



ABOUT PNNL

Pacific Northwest National Laboratory, a U.S. Department of Energy Office of Science laboratory, solves complex problems in energy, the environment, and national security by advancing the understanding of science. PNNL employs more than 4000 staff, has a business volume of $750 million, and has been managed by Ohio-based Battelle since the lab's inception in 1965.

For more information about the **Institute for Interfacial Catalysis**, contact:

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