Pacific Northwest National Laboratory

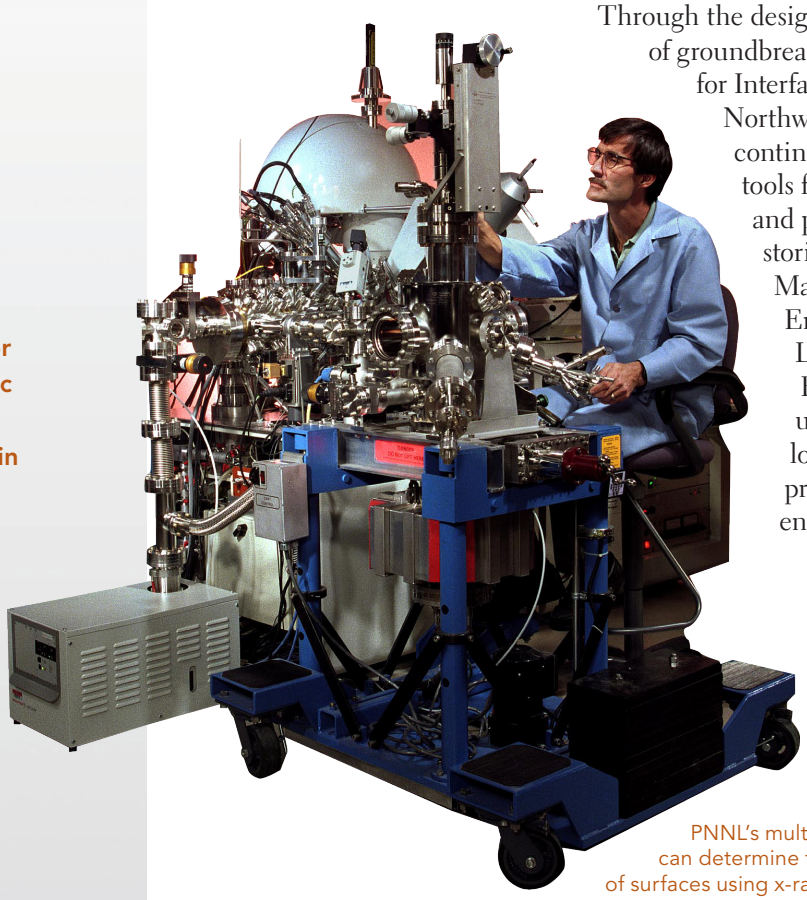
Pacific Northwest National Laboratory:

INSTITUTE FOR INTERFACIAL CATALYSIS

Experimental and Computational Capabilities for 21st Century Catalysis Research

Control of Chemical Transformations for a Secure Energy Future

- **PNNL continues to add to its broad portfolio of tools for research on catalytic materials and processes involved in producing, storing, transporting and using energy.**



PNNL's multi-technique surface analysis system can determine the composition and chemical nature of surfaces using x-ray photoelectron, Auger, ion-scattering and secondary ion mass spectrometry.

Through the design, development and deployment of groundbreaking capabilities, the Institute for Interfacial Catalysis (IIC) at Pacific Northwest National Laboratory (PNNL) continues to add to its broad portfolio of tools for research on catalytic materials and processes involved in producing, storing, transporting and using energy. Many of these tools are housed in the Environmental Molecular Sciences Laboratory, a U.S. Department of Energy (DOE) national scientific user facility at PNNL. Others are located in PNNL's physical sciences, process development and process engineering laboratories.

Catalytic systems are complex, and productive routes to new knowledge use complementary tools to deliver exquisite time, space and chemical resolution under conditions relevant for energy research.

UNDERSTANDING CATALYTIC REACTIONS

In catalytic systems, relevant time and length scales extend over orders of magnitude. The active sites of catalysts have nanometer, or smaller, dimensions and operate with atomic selectivity on time scales as short as a fraction of a femtosecond. On the other hand, measured catalytic reaction rates typically vary over longer times and larger lengths. We offer an extensive range of capabilities that cross these scales for both molecular and interfacial catalysis research.

Experimentally, reactor systems are central for studying thermal, electrochemical and photochemical catalysis. We offer a broad array including batch, continuous stirred and flow systems ranging from laboratory to mini-pilot plant scale. Among these are unique tools to measure a set of reaction rates—separated by no more than a few minutes—at vastly different pressures (10^{-9} Torr to 1000 psi). In concert with these reactors, we use tools for controlled preparation and characterization of catalysts and the reactions they facilitate. High priority is given to characterization of catalysts while functioning (*operando*).

U.S. DEPARTMENT OF ENERGY

We analyze new and used catalysts using element-sensitive optical spectroscopy and calorimetry and a host of electron and scanning probe structural tools (XRD, SEM, HR-TEM, EXAFS, STM and AFM). We analyze chemical properties optically (Raman and IR) and with a suite of electron and ion spectroscopies. Extensive NMR facilities, including an exquisite very high-field (900 MHz) system in EMSL, are exploited in our catalysis research.

CONTROLLING SYNTHESIS

Advances depend on controlled synthesis of new catalysts. We offer synthesis of molecular catalysts with exquisite control of ligands and synthesis of interfacial catalysts with control of structure, including porosity, across nanometer to micrometer length scales. To supplement traditional preparation procedures, we now offer self-assembly of controlled nanocrystals.

To synthesize model oxide catalysts in thin-film form, we offer state-of-the-art epitaxial growth capabilities.

COMBINATORIAL AND OPERANDO TOOLS

Among the recent additions to our experimental portfolio are several combinatorial and *operando* tools. The Combinatorial Catalyst Lab (Combicat) is an integrated system for high-throughput, including catalyst preparation and screening, and data visualization. A transient kinetic analysis tool probes steady-state mechanisms by analyzing transient responses of surface and gas phase species when an isotopically labeled reactant is replaced by one of its isotopomers. Also, we offer laboratory-scale, 1-atm reactors integrated with ultrahigh vacuum surface analysis tools for studying model systems.

Under development, Combocare combines combinatorial and *operando* measurements using real-time simultaneous Raman, IR imaging and GC mass spectrometry analysis of multiple catalysts for product analysis and catalyst characterization.

Future plans include acquiring a HR-TEM with an integrated, apertured, differentially pumped reaction cell for *in-situ* electron microscopy of the structure of functioning nanocatalysts.

LEVERAGING COMPUTATION RESOURCES

Experimental and theoretical research requires extensive computational resources. We use the world-leading hardware and software resources of the **EMSL Molecular Science Computing Facility** and other venues. For example, our computational catalysis capabilities include electronic structure and dynamics codes that examine atomic- and molecular-level events in thermal, photo- and electro-catalysis. We also use kinetic modeling codes that predict values for experimentally measurable reaction 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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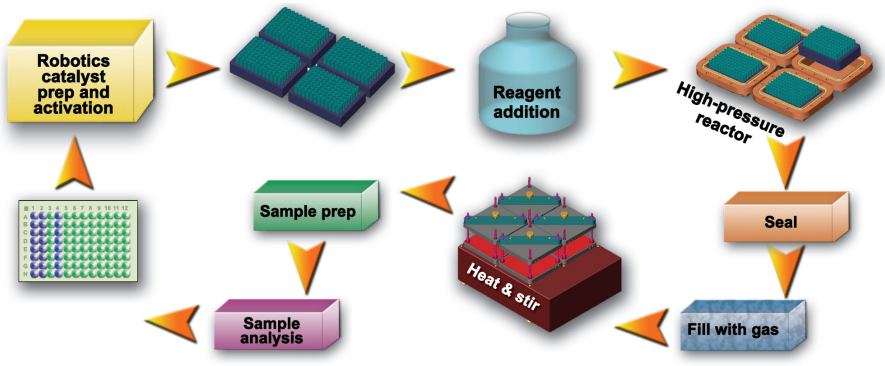

The CombiCat incorporates an integrated chemical analytical capability with a high-pressure liquid chromatography system, allowing 96 samples to be analyzed in less than 12 hours.

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