Pacific Northwest NATIONAL LABORATORY

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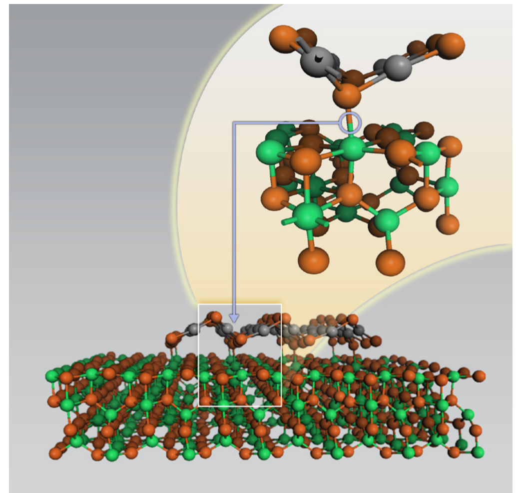
# Catalysis Research for Energy Independence

Chemical transformations are at the heart of energy production and use, and catalysis lies at the core of efficiently and effectively using our current energy sources, developing alternatives, and reducing environmental impacts. Practiced for more than a century, fundamental research into catalysts to enable desired reactions 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.



Research in *Science* reveals new, important details about platinum, a common catalyst; specifically, scientists showed how rafts of chemically reactive platinum form on oxide-based catalyst support materials. The new work yields insights into improving the industrial catalyst for oil refining, chemicals processing, and environmental applications.

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.

Research activities at Pacific Northwest National Laboratory's (PNNL's) Institute for Interfacial Catalysis and affiliated efforts are greatly advancing our ability to control chemical transformations and chemical-electrical energy inter-conversions to significantly reduce the carbon footprint of the global energy system.

In the Exhaust Emissions Science Laboratory, we investigate methods for reducing engine emissions from more fuel-efficient future vehicles.

We provide a fundamental understanding of catalytic materials and the chemical reactions occurring on catalyst surfaces and within the catalysts. Our fundamental research is primarily focused on converting biomass into fuels and value-added chemicals, converting carbon dioxide into fuels, and transforming electrical energy from renewable energy sources into chemical fuels.

In addition, we conduct applied catalysis research with industrial, academic, and other research entities. This work includes catalysis for upgrading biomass feedstock; for chemical energy storage, retrieval, and use; for emission control of fuel-efficient vehicles; and for the conversion of coal to fuels in an environmentally benign manner.

## INTERDISCIPLINARY LEADERSHIP

A critical mass of more than 90 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. Here is a selection of awards recently presented to our staff:

- **Charles H.F. Peden, Yong Wang, and Michel Dupuis,** American Association for the Advancement of Science Fellows
- **Gregory K. Schenter,** American Physical Society Fellow
- **Janos Szanyi,** Fulbright Fellowship
- **Bruce D. Kay,** American Chemical Society Fellow
- **Wendy Shaw,** U.S. Department of Energy Early Career Research Program Grant.

The Institute for Interfacial Catalysis draws upon a broad range of disciplines to create synergistic, interdisciplinary teams that include experimental and theoretical chemistry, physics, chemical and mechanical engineering, and materials science. We also collaborate with catalysis leaders in academia, industry, and national laboratories.

U.S. DEPARTMENT OF ENERGY

## FACILITIES

The Institute for Interfacial Catalysis uses leading-edge experimental and computational resources at the Environmental Molecular Sciences Laboratory, a U.S. Department of Energy national scientific user facility at PNNL. 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 at our collaborators' facilities.

Also located at PNNL is the Center for Molecular Electrocatalysis. The Center is developing a fundamental understanding of proton-transfer reactions that will lead to transformational changes in our ability to design molecules that catalyze the conversion of electrical energy into chemical bonds in fuels, and the reverse.

## SELECTED PUBLICATIONS


Appel AM, SJ Lee, JA Franz, DL DuBois, and M Rakowski DuBois. 2009. "Free Energy Landscapes for S-H Bonds in $Cp^*{}_2Mo_2S_4$ Complexes." *Journal of the American Chemical Society* **131**(14):5224-5232.

Kwak JH, J Hu, D Mei, CW Yi, DH Kim, CHF Peden, LF Allard, and J Szanyi. 2009. "Co-ordinatively Unsaturated $Al^{3+}$ Centers as Binding Sites for Active Catalyst Phases on $\gamma$-$Al_2O_3$." *Science* **325**(5948):1670-1673.

Mei D, RJ Rousseau, SM Kathmann, VA Glezakou, MH Engelhard, W Jiang, CM Wang, MA Gerber, JF White, and DJ Stevens. 2010. "Ethanol Synthesis from Syngas over Rh-based/$SiO_2$ Catalysts: A Combined Experimental and Theoretical Modeling Study." *Journal of Catalysis* **271**(2):325-342.

Mock MT, RG Potter, DM Camaioni, J Li, WG Dougherty, WS Kassel, B Twamley, and DL DuBois. 2009. "Thermodynamic Studies and Hydride Transfer Reactions from a Rhodium Complex to $BX_3$ Compounds." *Journal of the American Chemical Society* **131**(40):14454-14465.

Zhang S, Y Shao, G Yin, and Y Lin. 2010. "Electrostatic Self-Assembly of Pt-around-Au Nanocomposite with High Activity towards Formic Acid Oxidation." *Angewandte Chemie International Edition* **49**(12):2211-2214.

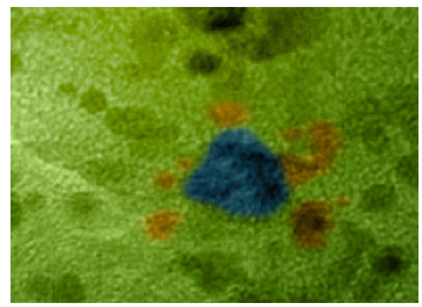

## OPPOSITES ATTRACT AND INSPIRE ELECTROCATALYST

### U.S., China team to convince platinum and gold particles to come together and form highly active nanocatalysts

Tiny gold particles will surround themselves with even smaller platinum bits, creating a complex structure that could turn a common preservative, formic acid, into electricity in a fuel cell, according to scientists from China's Harbin Institute of Technology and PNNL. The team used a novel electrostatic self-assembly method to create platinum-surrounded gold nanomaterial. This method relies on the attraction between positive and negative charges to inspire nanoparticles to form new structures on their own.

"To our knowledge, this is the first time that this method has been used to create such catalysts," said Dr. Yuehe Lin, a chemist at PNNL and a co-corresponding author of the paper. This paper was named a Very Important Paper by *Angewandte Chemie International Edition*. Less than 5% of the journal's manuscripts receive such a positive recommendation, and this was the only one in the current issue.

Replacing today's batteries in laptop computers and other portable devices with liquid fuel-powered fuel cells could ease consumer frustrations. The fuel cells would last 2 to 10 times as long as today's batteries. Further, the laptop computer could be recharged instantly, because it relies on formic acid, not electricity. In addition, this kind of fuel cell can be used as a battery-electric vehicle range extender if assembled into a stack. But, such fuel cells must have efficient catalysts to create the needed power. This research provides fundamental insights into designing such catalysts.



Gold particles (colored in blue) will surround themselves with even smaller platinum particles (colored in orange), creating a structure that could turn a common preservative into electricity in a fuel cell, according to a study by scientists at China's Harbin Institute of Technology and PNNL.

## 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 4,600 staff, has a business volume exceeding $800 million, and has been managed by Ohio-based Battelle since the Lab's inception in 1965.

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Institute for INTERFACIAL CATALYSIS