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By taking an integrated approach to catalysis, researchers at Pacific Northwest National Laboratory's Institute for Integrated Catalysis are helping to change how fuels are produced and used.





# INSTITUTE FOR INTEGRATED CATALYSIS 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, catalysis research to enable desired reactions is being newly invigorated by advances in capabilities to make, measure, and model the chemical and physical properties accurately and with exquisite spatial and temporal detail. The grand scientific challenge is to understand how to design catalyst structures to *control activity and selectivity*, and then put this understanding to use.

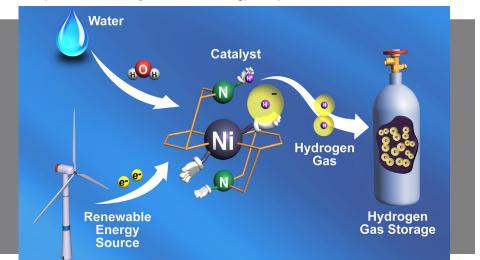
Research activities at Pacific Northwest National Laboratory's Institute for Integrated Catalysis and affiliated efforts are greatly advancing our ability to control chemical transformations and chemical-electrical energy inter-conversions to create a sustainable global energy system.

We provide a fundamental understanding of catalytic materials and the chemical reactions occurring on catalyst surfaces and within the catalysts. In addition, we conduct applied research with industrial, academic, and other research entities. This work includes catalysis for upgrading biomass feedstocks; for chemical energy storage, retrieval, and use; and for emission control of fuel-efficient vehicles.

## Interdisciplinary Leadership

A critical mass of approximately 150 scientists and engineers in the IIC contribute to catalyst-related research. These researchers create synergistic, interdisciplinary teams that include experimental and theoretical chemistry, physics, chemical and mechanical engineering, and materials science. Many of these staff are widely recognized in the external community. Recent awards include

- Johannes Lercher, 2011 Robert Burwell Lecturer by the North American Catalysis Society
- Charles H.F. Peden, Yong Wang, Michel Dupuis and Gregory K. Schenter, American Association for the Advancement of Science Fellows
- ▶ Bruce D. Kay and Yong Wang, American Chemical Society Fellows
- ▶ Wendy Shaw, U.S. Department of Energy Early Career Research Grant.



Looking to nature for their muse, researchers at Pacific Northwest National Laboratory have used a common protein to guide the design of a material that can make energy-storing hydrogen gas. The synthetic material works 10 times faster than the original protein found in water-dwelling microbes, the researchers report in the August 12 issue of Science, clocking in at 100,000 molecules of hydrogen gas every second.

### **Selected Publications**

Helm ML, MP Stewart, RM Bullock, M Rakowski DuBois, and DL DuBois. 2011. "A Synthetic Nickel Electrocatalyst With a Turnover Frequency Above 100,000 s<sup>-1</sup> for H<sub>2</sub> Production." *Science*, August 12, 2011.

Bullock RM. 2011. "A Mercurial Route to a Cobalt Dihydrogen Complex." *Angewandte Chemie International Edition* **50**(18):4050-4052.

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<sub>2</sub> Catalysts: A Combined Experimental and Theoretical Modeling Study." *Journal of Catalysis* **271**(2):325-342.

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.

Kwak JH, J Hu, D Mei, CW Yi, DH Kim, CHF Peden, LF Allard, and



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.

## **Researchers Work Around the World**

Our researchers work with academic institutions, research agencies, and private industry around the world. Here are a few examples:

- Albemarle Corporation
- Archer Daniels Midland Company
- Argonne National Laboratory
- Caterpillar
- Chinese Academy of Sciences
- Cummins Inc.
- Dalian Institute for Chemical Physics in China
- Dow Automotive
- Fritz-Haber Institute in Germany
- General Electric
- General Motors
- InnovaTek
- LanzaTech
- Lawrence Berkeley National Laboratory
- Los Alamos National Laboratory
- Louisiana State University
- Nanjing Normal University in China

- National Energy Technology Laboratory
- Oak Ridge National Laboratory
- Princeton University
- Sungshin Women's University, Korea
- University of Connecticut
- University of Delaware
- University of Minnesota
- University of Missouri-Columbia
- University of New Mexico
- University of Pennsylvania
- University of Texas at Austin
- University of Toronto
- University of Washington
- UOP LLC
- Washington State University

J Szanyi. 2009. "Co-ordinatively Unsaturated Al<sup>3+</sup> Centers as Binding Sites for Active Catalyst Phases on γ-Al<sub>2</sub>O<sub>3</sub>." *Science* **325**(5948):1670-1673.

### Patents

Catalysis research from the IIC has earned 8 U.S. patents this year. Since 2001, we have received 105 U.S. and foreign patents.

# **ABOUT PNNL**

Pacific Northwest National Laboratory is a Department of Energy Office of Science national laboratory where interdisciplinary teams advance science and technology and deliver solutions to America's most intractable problems in energy, the environment and national security. PNNL employs 4,900 staff, has an annual budget of nearly \$1.1 billion, and has been managed by Ohio-based Battelle since the lab's inception in 1965. Follow PNNL on Facebook, LinkedIn and Twitter.

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