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Cracking the catalytic code

April 25 2018, by Steve Koppes

Credit: Argonne National Laboratory

The newly developed ability to tap previously inaccessible shale gas deposits during the last decade has created an abundant source of gases, including methane, ethane and propane, that are used to create chemicalbased products such as plastics. But the U.S. chemical industry needs scientists, including those at the U.S. Department of Energy's (DOE) Argonne National Laboratory, to help turn that new feedstock supply into a competitive technological advantage.

In a variety of research programs, Argonne experts are finding ways to more cheaply and efficiently manufacture products derived from shale gas deposits and are identifying new routes to make higher-performance catalysts.

"In order to maximize the benefits and take advantage of today's inexpensive source of natural gas and natural gas liquids to create investments and jobs in the United States, it is important to develop new and more efficient processes related to catalytic conversion of natural gas to higher-value materials," asserted a 2016 report of the National Academy of Sciences.

Shale gas is a natural gas found in shale rock formations created hundreds of millions of years ago. The wet part of shale gas contains a variety of alkanes, a family of commercially important hydrocarbons that includes ethane and propane. The chemical industry is interested in alkanes that can be converted into alkenes—a class of hydrocarbons useful in manufacturing a variety of materials, mostly polymers such as polyethylene and polypropylene. Argonne's catalysis science program has already developed a successful method for effectively converting alkanes to alkenes. Now, the researchers also investigate how they can make other compounds of interest to the chemical industry.

"The goal is to understand how to manipulate single-site catalysts on surfaces and how we can achieve high selectivity for light alkane transformation to added-value products such as olefins, which have found widespread use in the manufacturing industry," said Max Delferro, an Argonne chemist who leads the laboratory's catalysis group.

Argonne scientists focus much of their work on single-site catalysts because of the promise they show for both high activity and product selectivity. Such work has resulted in two U.S. patent applications for the development of multi-metallic catalysts that selectively dehydrogenate n-butane to 1,3-butadiene (BDE). BDE is a primary building block of synthetic rubber, which polymer manufacturers have used to make car tires.

Current process technologies for converting alkanes to alkenes all involve coking, a carbon-deposition process that interferes with catalytic activity. "The problem with coking is that you're not converting your feedstock to the product you want. You're converting it to a byproduct," said Ted Krause, a chemical engineer and department head in Argonne's Chemical Sciences and Engineering division. Argonne's single-site catalyst technology dehydrogenates alkanes without promoting coking.

The work targets a range of catalysts and reactions from which private companies might select for optimization and commercialization. "One of the main goals is to transfer the knowledge from the basic energy sciences side to the markets," said Delferro.

Krause leads a second project, funded through DOE's Office of Energy Efficiency and Renewable Energy (EERE) Bioenergy Technologies Office. In this project, researchers use X-ray spectroscopy at the Advanced Photon Source (APS), a DOE Office of Science User Facility, to understand how catalysts react and how they deactivate.

Argonne's catalysis scientists are working with several companies in the biofuels and biochemical industry through cooperative agreements to spur the development of catalytic materials. In APS experiments, Argonne researchers probe catalytic reactions with an X-ray beam to monitor the changes that catalysts undergo during actual working conditions.

Catalysis science has been an APS mainstay since the APS began operation in 1996. In situ and operando experimentation capabilities are an important strength of the APS, enabling measurements under real-world conditions, said Greg Halder, business development executive in Argonne's Technology Commercialization and Partnerships division.

"These approaches span a suite of beamlines that allow industry to watch reactions happen in real time and measure catalytic performance by precisely monitoring a range of chemical and physical properties," Halder said. "This information can then be combined with experimental and computational data and expertise to develop the next generation of catalysts."

Argonne researchers specialize in understanding why catalysts deactivate—why they die—and in developing techniques to mitigate that process.

"Catalyst lifetime is a critical cost factor," Krause said. "If it's short, you need a regeneration process, because the cost of exchanging it with fresh catalyst could be prohibitive. Even for long-term catalysts, as they begin to deactivate with time, you tend to lose selectivity to the desired product, so you tend to make less of your desired product."

Chris Marshall, a senior research chemist in the catalysis group, leads a DOE EERE Advanced Manufacturing Office-funded project to develop capabilities for extending catalyst lifetime. "We've developed techniques for stabilizing catalysts, particularly under harsh reaction conditions," Krause said.

In addition to its expertise, Argonne is equipped with infrastructure that accelerates the discovery of both materials and process conditions. The laboratory's catalyst tool for atomic layer deposition synthesis offers precise control over the process at the atomic level, and Argonne's highthroughput robotic synthesis platform screens multiple catalysts simultaneously for a wide variety of reactions and reaction conditions.

Provided by Argonne National Laboratory