Researchers discover less expensive low-temperature catalyst for hydrogen purification

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(PhysOrg.com) -- Engineering researchers from Tufts University, the University of Wisconsin-Madison and Harvard University have demonstrated the low-temperature efficacy of an atomically dispersed platinum catalyst, which could be suitable for on-board hydrogen production in fuel-cell-powered vehicles of the future.

An alternative to copper, which under certain conditions can ignite spontaneously, the platinum-based catalyst is highly active and stable. The researchers' understanding of the structure and function of the new catalyst could help manufacturers design highly effective—but less costly—catalysts on standard, inexpensive support metal oxides.

Led by Maria Flytzani-Stephanopoulos, a Tufts University School of Engineering professor of chemical and biological engineering, and Manos Mavrikakis, a UW-Madison professor of chemical and biological engineering, the research team published its findings in the Sept. 24, 2010, issue of the journal *Science*.

Only small amounts of hydrogen occur naturally on Earth—yet, according to the U.S. Department of Energy, the country's demand for hydrogen is about 9 million tons per year.

Manufacturers produce about 95 percent of this hydrogen through steam reforming of natural gas, a catalytic process in which steam reacts with methane to yield carbon monoxide and hydrogen. This mixture is known as synthesis gas, or syngas, and is an intermediate in production processes for synthetic fuels, ammonia and methanol, among other compounds.

Another application for hydrogen is fuel for the hydrogen economy, an effort that aims to exploit high-energy-density hydrogen as a cleaner source of energy, particularly for low-temperature fuel-cell-powered devices, including vehicles.

Fuel cells use electrochemical processes to convert hydrogen and oxygen into water, producing direct current that powers a motor. Fuel cell vehicles require highly purified hydrogen, which is produced through a water-gas-shift reaction. This key step strips "residual" carbon monoxide from hydrogen generated through steam reforming of fossil fuels, such as natural gas. Water-gas-shift catalysts decrease the amount of carbon monoxide in hydrogen and increase the hydrogen content by harvesting hydrogen from water molecules.

Catalysts currently used in industry for hydrogen purification are copper-based, supported on zinc oxide and alumina. Because copper is pyrophoric (it could spontaneously ignite when exposed to air; air in fuel cell operation is relatively common), researchers have considered platinum as a substitute. However, platinum is costly and, says Flytzani-Stephanopoulos, researchers must prepare it in very fine particles on more "exotic" supports, such as the rare-earth oxide ceria, which makes it effective for a low-temperature water-gas-shift reaction.

However, while cerium is the most abundant of the rare-earth elements, this natural abundance occurs in just a few places around the world, and, says Mavrikakis, access to it may be limited for various reasons, including geopolitical.

The Tufts researchers initially discovered that sodium improves the platinum activity in the water-gas-shift reaction, which now can take place at low temperatures, even on inert materials like silica. They carried out detailed structural studies and found extra active oxygen species on the surface that helped the platinum complete the reaction cycle. They also found that the sodium or potassium ions helped to stabilize the catalytic site.

In later experiments, they saw their catalyst perform as well as platinum on ceria. Collaborator David Bell of Harvard University used atomic-resolution electron microscopy to view stabilized platinum clusters and atoms on the silica support—visual confirmation that the new catalyst operates like those on ceria supports.

Mavrikakis' team set out to understand why. The researchers drew on powerful computational resources, including the UW-Madison Division of Information Technology and the Center for High-Throughput Computing, as well as an ultrafast 10G data network, to model the new catalyst, atom by atom. "There is no experimental way that you can look at the atoms 'at work'—that is, while the reaction is happening," says Mavrikakis. "You need to start talking about individual atoms, which you can see with the highest-resolution electron microscopes—but not during the reaction. So you can only suggest that perhaps these atoms are active, but there is no way to substantiate it unless you put an atomic-scale quantum-mechanical model together and come up with a more realistic and well-founded suggestion about what is responsible for making this catalyst so active."

Although platinum is among the most expensive catalytic materials, the new catalyst contains only trace amounts of platinum, yet is robust and effective at low temperatures. Essentially, its structure is a series of small "clusters" comprising only a few atoms, each in a specific arrangement. Each cluster is composed of one or a few a platinum atoms surrounded by a mixture of oxygen, hydroxyl and potassium atoms and is "seated" on the standard aluminum or silica support.

The researchers say the advance is important in part because, through a combination of experiments and first-principles theory, the work reveals a new type of active site for a specific, very important chemical reaction. "Most of the time, people are happy to say, 'Well, we've found a material. It works for a given application,'" says Mavrikakis.

In this case, says Flytzani-Stephanopoulos, the team took the next step to determine how and why the catalyst works. "If we want to move to the next stage with cheaper materials that are doing the specific chemical transformations, we need to understand the fundamentals," she says.

Provided by University of Wisconsin-Madison

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