

## Purdue finding could help develop clean energy technology

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Chemical engineers at Purdue University have made a discovery that may help to improve a promising low-polluting energy technology that combusts natural gas more cleanly than conventional methods.

The finding revolves around the fact that catalysts and other materials vital to industry have complex crystalline structures with numerous sides, or facets. Different facets sometimes provide higher performance than others, so industry tries to prepare catalytic materials that contain a large number of higher-performing facets.

The Purdue researchers have determined, however, that the precious metal palladium, the catalyst used in the clean energy technology – called catalytic combustion – performs the same no matter which facet is exposed.

"Palladium is the best metal for the catalytic combustion of methane, which is contained in natural gas," said Fabio Ribeiro, an associate professor of chemical engineering at Purdue. "There is no other element in the periodic table you can use that's better than palladium for this reaction."

To produce electricity, natural gas is burned in a turbine similar to a jet engine, and the turbine runs a generator. The conventional method, which is widely used in commercial power generation, burns natural gas with a flame. Researchers are trying to eliminate the flame, replacing it with a catalyst that combusts methane at lower temperature, emitting less smog-producing nitrogen oxide pollution. The catalytic combustion



technology is promising as a future energy source because it generates less pollution without losing efficiency, but industry is still trying to find higher-performance catalysts to improve the process.

The research findings are detailed in a paper presented today (Tuesday, March 15) during a meeting of the American Chemical Society in San Diego. The paper was written by Ribeiro; Jinyi Han, a researcher from Worcester Polytechnic Institute in Massachusetts; Purdue postdoctoral student Guanghui Zhu; and Dmitri Y. Zemlianov, a researcher from the University of Limerick in Ireland.

Catalysts are critical for numerous manufacturing processes and everyday applications, such as a car's catalytic converter. Industry prepares tiny catalyst clusters only a few nanometers, or billionths of a meter, in diameter that contain numerous facets. The clusters are then coated on a spongelike, porous "support material."

"Because the support material is porous, it has a larger overall surface area than a smooth material would have, making it possible to increase the amount of catalyst per unit of volumepresent and boosting performance," Ribeiro said.

Another way to increase performance is to find which facets work best. The composition of the catalyst is the same in each facet, but the arrangement of atoms is different, much like the way in which a pile of oranges can be arranged in many different ways.

"Some piles will have square shapes, others will be hexagonal, others will have different kinds of troughs, or spacing, between rows of oranges," Ribeiro said. "What we want to know is whether the arrangement on the surface will make a difference. If industry researchers want to prepare catalysts, they want to know whether it matters if they use small particles, big particles, a particle that has a certain shape on its surface,



and so on. Suppose I find out that, for a certain reaction, one of the facets is much better than all the others – perhaps as much as a thousand times better? And there are cases where that is true. Then I can tell the people who make that catalyst that only this facet is important."

If a particular facet is known to perform better than others, industry prepares clusters that contain a large number of those facets.

Finding the best facet, however, is difficult because commercial catalyst clusters contain a complex combination of many different facets.

"Each of these clusters can be very different, or non-uniform, from one place to another, which makes it difficult to pick out individual facets," Ribeiro said. "It's like a million people screaming at the same time. You can't distinguish one person's voice from the next.

"It's very difficult to learn exactly how a catalyst works by studying these non-uniform particles. All you can really do is get an average performance for all of the different facets combined. But we want to learn precisely how each separate facet performs."

The engineers do that by using a large single crystal, cutting it at the proper angle with special equipment, and then polishing the surface to a mirror finish, creating pieces about 1 centimeter in diameter that expose only a particular configuration of atoms.

"I can now simplify the problem by studying just one facet at a time for this particular reaction."

Samples have to be prepared under ultra-high vacuum – a millionth of a millionth of Earth's normal atmospheric pressure – so that they are not contaminated by impurities. After being cleaned, the samples are transferred to a chamber where the chemical reactions can be studied at



regular pressure.

Determining how well a catalyst works requires engineers to precisely duplicate the same conditions in which the catalysts are used.

"You must recreate the same temperature and the same concentration that the real catalyst sees so that you measure the rate at exactly the same conditions," Ribeiro said. "And then we can measure the rates and say, 'That's the maximum you will ever get from your catalyst.' So we tell industry that this is the benchmark for a certain catalyst."

The Purdue researchers used the method to study the oxidation of methane on a palladium catalyst, a reaction that is critical to the catalytic combustion of natural gas.

"What we are saying here is that, in this case, no matter what surface you have exposed, no matter what size the particles are or anything like that, the rate is always the same. So don't spend your time trying to make something that has a certain shape because it doesn't matter.

"If researchers want a rate beyond what is currently possible with palladium, they need to find a totally different catalyst."

The research has been funded by the U.S. Department of Energy, and Ribeiro's lab is associated with the Birck Nanotechnology Center in Purdue's Discovery Park, the university's hub for interdisciplinary research. The research is ongoing and is supported by Purdue's recently formed Center for Catalyst Design.

Source: Purdue University



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