Researchers uncover basics of common industrial catalytic processes

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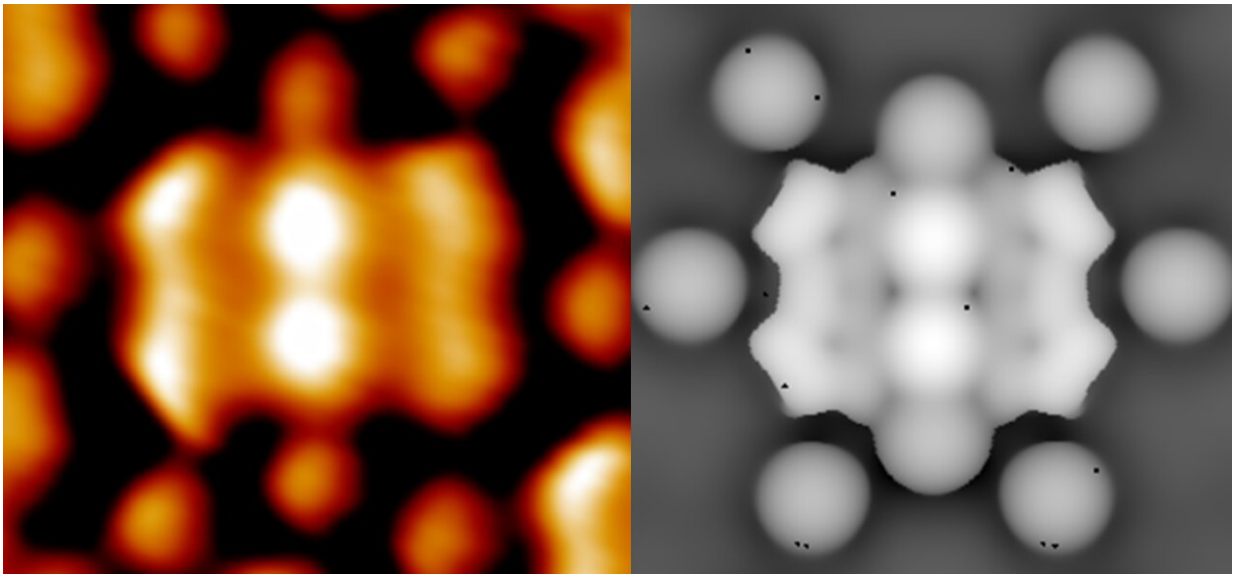

The images compare experimental (left) and simulated (right) reaction intermediate in the formation of a benzene-like compound with single bonds. Credit: Washington State University

Catalysts are used in a wide variety of industrial processes around the world in everything from the production of medicines, fertilizers, plastics, and other household products to the processing of fossil fuels.

They speed up chemical reactions with the aim of minimizing energy usage. But while they are critically important, catalysts have often been

developed through trial and error or tradition rather than through scientific principles.

Using a combination of microscopy and spectroscopy to get real-world imagery as well as sophisticated theoretical calculations, Washington State University researchers collaborated with Prof. Junfa Zhu from the University of Science and Technology of China to unravel an underlying mechanism of a catalytic reaction at the atomic level.

The work, published in the journal of the American Chemical Society, *JACS*, improves fundamental understanding of reactions that could someday lead to more efficient industrial processes.

"There's a popular image of something like witch's brew in which things are randomly stirred together to make the catalysts what they are. Here we're trying to predict how to synthesize something very particular," said Jean-Sabin McEwen, associate professor in the Gene and Linda Voiland School of Chemical Engineering and Bioengineering and corresponding author on the paper.

The researchers studied the reactions of a chemical called biphenyl, a naturally occurring organic compound that is in coal, natural gas, and crude oil. The researchers compared two slightly different versions of the chemical. Adding two or four extra bromine atoms to the molecule resulted in a dramatically different chemical reaction when they interacted with a simple silver surface. In one case, the result was a benzene-like compound with single bonds. In the other, the molecule resembled a honeycomb, similar to the beginning of a carbon graphene sheet. One of the reactions also required higher temperatures and more energy to complete, an important concern for industries using catalytic reactions. The researchers were able to match atomic scale images of the reaction they observed with theoretical calculations.

"In real catalysts, when there are so many side reactions, it's so complicated that making the direct link between experiment and theory is very difficult," McEwen said. "But when you have well-defined catalysts like those we were looking at, you can obtain a much more predictive understanding of what's going on, and this can be used as a stepping stone toward the development of more complex models on more realistic catalytic surfaces."

WSU recently became an affiliate member of the Center for Rational Catalyst Synthesis, a National Science Foundation-funded center that aims to better understand the fundamentals of making catalysts. The NSF center asks that universities work with industrial partners in an effort to solve real-world problems, said McEwen.

Developing catalysts is very costly for industries, requiring systematic and repeated testing that have great difficulty in predicting end results, he said.

"It would be a huge saving in cost if we could predict what we're going to get at the end of the day, either computationally or through a combination of experiments and theory," he said. "This is a very fundamental study that addresses the interest of industries in making catalysts what they are."

More information: Zhiwen Zeng et al, Chemisorption-Induced Formation of Biphenylene Dimer on Ag(111), *Journal of the American Chemical Society* (2021). DOI: 10.1021/jacs.1c08284

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