Study could lead to improved catalysts for producing hydrogen fuel from waste biomass

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Experimental analysis and computer simulations reveal new insights into the process by which ethanol produced from waste biomass can be converted into hydrogen in the presence of a catalyst. These insights should aid the design of more efficient catalysts for hydrogen production.

Hydrogen gas is an environmentally friendly alternative to fossil fuels. Today, through a process known as steam reforming, hydrogen is obtained by using steam to break up a hydrocarbon—most commonly, methane in natural gas. However, ethanol produced by fermenting waste biomass is potentially a cleaner starting material for this process.

However, despite having been extensively studied in recent years, steam reforming of ethanol is currently too inefficient to produce hydrogen on an industrial scale. This stems partly from the complexity of its reaction, which can yield a range of different products. "Our lack of understanding of the detailed reaction mechanism hinders further improvement of a catalyst for the reaction," explains Jia Zhang of the A*STAR Institute of High Performance Computing in Singapore. "The reaction was a black box before we started exploring it."

Now, Zhang and her co-workers have used experiments and computer simulations to probe how ethanol breaks down into hydrogen on rhodium catalysts supported on zirconia-based oxides. These nanosized catalysts had previously been shown to be highly active for this reaction.

The team used gas chromatography and mass spectrometry to monitor in real time the intermediate species that form as the reaction proceeds. These measurements revealed that the C2H4O species is an important intermediate. Of the two possible structures this species can adopt, acetaldehyde (CH3CHO) was identified as the most probable one by the team's computer calculations. The calculations also showed that water plays an unexpectedly important role in controlling the reaction pathway.

Based on this knowledge, the team proposed a mechanism for the reaction under their chosen conditions. Hydrogen is produced at most stages along the pathway, including the final step in which carbon monoxide reacts with water to produce hydrogen and carbon dioxide. The team's calculations showed that the success of this final step is critical in determining the amount of hydrogen produced by steam reforming.

"Our theoretical simulations and experimental analysis provide important information on the reaction mechanism," says Zhang. "This is a fundamental step forward in our understanding of the catalyst, which is the basis of catalyst design." The team's ultimate goal is to design catalysts that can produce hydrogen more cheaply and efficiently than current catalysts.

More information: Zhang, J., Zhong, Z., Cao, X.-M., Hu, P., Sullivan, M. B. & Chen, L. Ethanol steam reforming on Rh catalysts: Theoretical and experimental understanding. *ACS Catalysis* 4, 448–456 (2014). dx.doi.org/10.1021/cs400725k

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