

Computer simulations reveal how rhodium catalysts structures break ethanol molecules into hydrogen atoms

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Hydrogen gas (H₂) is an ideal energy carrier for fuel cells, but finding sustainable ways to produce large quantities of hydrogen continues to be a technological challenge. Jia Zhang at the A*STAR Institute of High Performance Computing and co-workers have now used sophisticated

calculations to uncover a critical chemical mechanism that may make catalytic transformation of safe, renewable liquid ethanol into hydrogen fuel easier than ever before.

Currently, steam reforming is the popular method for producing [hydrogen gas](#) from [ethanol](#). In this technique, ethanol is injected into a hot, steam-filled chamber containing a catalyst such as rhodium. The catalyst promotes the dissociation of ethanol molecules into smaller molecules, such as carbon monoxide and H₂. Although chemists have had good success in using steam reforming to ‘crack’ ethanol, they have had difficulties in improving the efficiency of the catalyst because of the many diverse and complex chemical reactions at play in the system.

According to Zhang, catalysts need to selectively crack the carbon–carbon bonds of surface-adsorbed ethanol to be viable for steam reforming. Recent experimental efforts have shown that ‘stepped’ catalyst surfaces — tiny staircase-like defects present in a normally flat rhodium surface — are unusually active at both carbon-hydrogen and carbon–carbon bond cleaving. One problem, however, is that the actual mechanism of ethanol decomposition on stepped surfaces is still unclear.

The research team overcame this challenge by using high-powered computer simulations to work out which ethanol decomposition pathways are most probable on a particular stepped rhodium surface known as rhodium (211). Exhaustive calculations using density functional theory (DFT) methods revealed that there were two ways of breaking ethanol down into H₂, and both shared a common intermediate species with the chemical formula CH₃COH.

Crucially, the team found that this CH₃COH intermediate exists only on stepped rhodium surfaces. While flat catalyst surfaces fracture ethanol through an oxametallacycle intermediate, the step-type defects preferentially absorb the alcohol and then activate the decomposition

cycle by sequentially removing hydrogen atoms from the intermediate. The researchers note that the surface-sensitivity of ethanol steam reforming is an important finding because step-defects are extremely common on state-of-the-art nanoscale rhodium catalysts.

“Steam reforming is a very complicated chemical process, and our current DFT study on ethanol decomposition mechanism is just the tip of the iceberg — many factors such as temperature, concentration, substrate influence, and water effects can influence the results,” says Zhang. “However, this work is an important first step for establishing theoretical rules to guide development of new, high-performance catalyst materials.”

More information: Zhang, J. et al. Density functional theory studies of ethanol decomposition on Rh(211). *Journal of Physical Chemistry C* 115, 22429–22437 (2011). [dx.doi.org/10.1021/jp206837z](https://doi.org/10.1021/jp206837z)

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