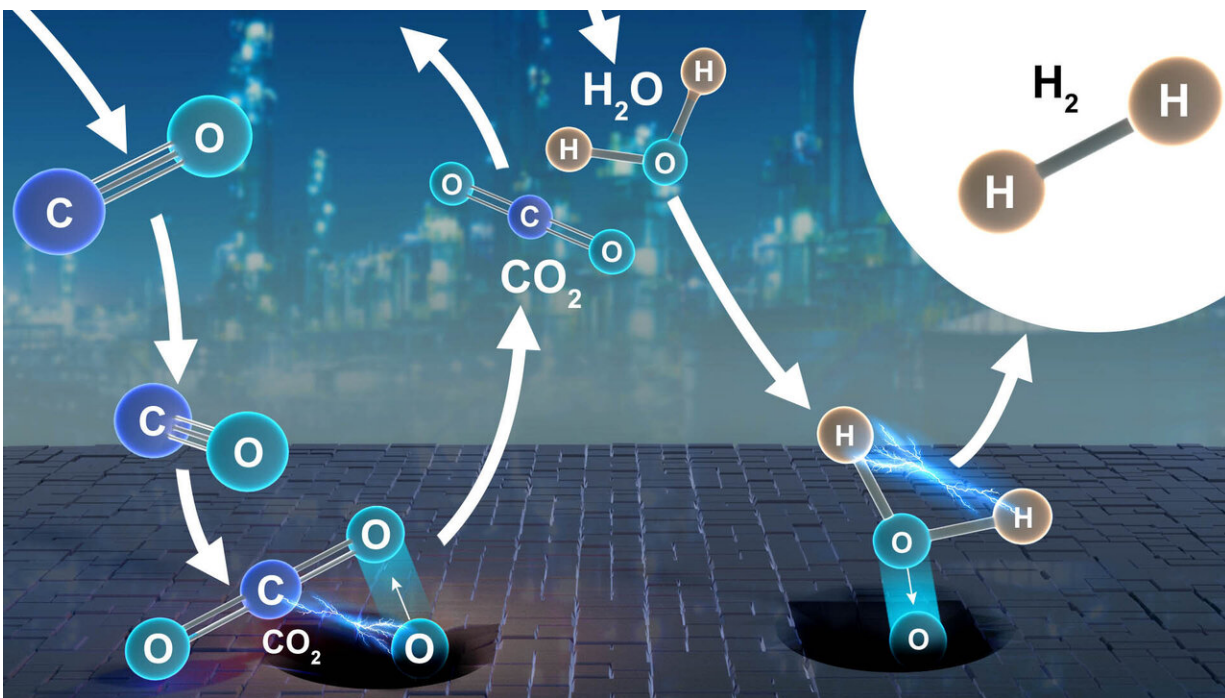


Neutrons shed light on industrial catalyst for hydrogen production

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Collaborators at the Department of Energy's Oak Ridge National Laboratory and U.S. universities used neutron scattering and other advanced characterization techniques to study how a prominent catalyst enables the “water-gas shift” reaction to purify and generate hydrogen at industrial scale. Credit: Oak Ridge National Laboratory

Collaborators at the Department of Energy's Oak Ridge National Laboratory and U.S. universities used neutron scattering and other

advanced characterization techniques to study how a prominent catalyst enables the "water-gas shift" reaction to purify and generate hydrogen at industrial scale.

Results published in the *Journal of the American Chemical Society* settled a long-standing debate about the catalyst's reaction mechanism, opening routes to improve the cost and efficiency of large-scale hydrogen production.

"Our work significantly advances fundamental understanding of a complex, industry-critical catalyst that has been difficult to study," said Zili Wu of ORNL's Chemical Sciences Division. "Determining how this reaction works at the atomic level enables further efforts to optimize the catalyst for improved performance."

Collaborators investigated a copper-chromium-iron oxide catalyst (CuCrFeO_x) provided by Lehigh University.

"We already know the existing CuCrFeO_x catalyst works, but how it works has been the subject of debate," said ORNL's Felipe Polo-Garzon, who worked with Wu on the team's multimodal approach to pinpoint the catalyst's reaction mechanism.

The goal was to study how the catalyst behaves in real-world conditions to find evidence of either an oxidation-reduction ("redox") or an associative mechanism—two predominant theories about how CuCrFeO_x works to produce hydrogen.

In a redox reaction, reactants exchange some of their atoms with the catalyst's surface to yield new substances, in this example, hydrogen and carbon dioxide. By contrast, in an associative reaction, all the reacting molecules bond to the catalyst's surface in an intermediate step to arriving at the final products.

To prove unambiguously how the CuCrFeO_x catalyst works (redox vs. associative mechanism), researchers cast a wide net of experimental and computational methods.

All results pointed to the same conclusion—a redox reaction. At high-temperature conditions, the catalyst loses oxygen atoms to make room for water molecules that dissociate and give off pure hydrogen.

"The answer is important because it helps us identify the critical point in the reaction where hydrogen is generated," said Polo-Garzon.

Many existing catalysts have been created through trial and error, which often limits their efficiency. The team's fundamental discovery could eliminate guesswork and tell researchers precisely where to look for opportunities to synthesize a better catalyst for generating hydrogen.

Hydrogen is the earth's most abundant element, but it does not occur naturally in the pure form needed by industries for oil refining, ammonia production for fertilizers, food processing, metal treatment, and other broad applications. Most of the world's hydrogen supply is produced by steam methane reforming—converting natural gas into a hydrogen mixture that is refined via water-gas shift catalysis to make pure hydrogen.

Several factors limit the understanding of what makes hydrogen generation possible during the [water-gas shift reaction](#). The CuCrFeO_x catalyst reconstructs during operation, so the fresh and spent versions are different, making it especially challenging to characterize the material. Previously, information about how the surface chemistry changes during reaction conditions has been missing from the puzzle.

Another hurdle is the compound's color. The black catalyst obstructs [optical spectroscopy](#) and other conventional techniques that rely on light

to obtain data, because the sample is too dark to "see" effectively.

Neutron vibrational spectroscopy experiments performed on the VISION beamline at ORNL's Spallation Neutron Source, a DOE Office of Science User Facility, helped overcome some of the challenges of studying CuCrFeO_x .

Because neutrons interact with samples differently than light does, they can complement information obtained from optical techniques. They are also ideal for observing hydrogen, which is difficult to detect with other experimental methods because of the element's low atomic weight.

The payoff was two-fold, says Polo-Garzon. "Neutrons gave us a critical piece of the puzzle to disprove the associative mechanism, showing us that no relevant intermediate was present on the catalyst's surface," he said. "We also observed something that has not previously been detected on the [catalyst](#)'s surface—hydrides."

Hydrides are surface species that play a key role in [hydrogen](#)-based reactions but are extremely difficult to observe in mixed-metal materials like CuCrFeO_x .

In addition to neutron experiments, researchers performed infrared spectroscopy and temperature-programmed surface reaction characterization at the Center for Nanophase Materials Sciences, a DOE Office of Science User Facility, and isotopic transient kinetic analysis at ORNL; near-ambient pressure X-ray photoelectron spectroscopy at the University of Kansas; and density functional theory calculations at the University of California, Riverside, which used resources of the National Energy Research Scientific Computing Center, a DOE Office of Science User Facility.

"You need more than one approach to gather and interpret all of the

information needed to build the whole story," said Polo-Garzon. "Our collaboration highlights the success of a multimodal approach to yield fundamental breakthroughs."

The journal article is published as "Elucidation of the Reaction Mechanism for High-Temperature Water Gas Shift over an Industrial-Type Copper–Chromium–Iron Oxide Catalyst."

More information: Felipe Polo-Garzon et al. Elucidation of the Reaction Mechanism for High-Temperature Water Gas Shift over an Industrial-Type Copper–Chromium–Iron Oxide Catalyst, *Journal of the American Chemical Society* (2019). [DOI: 10.1021/jacs.9b03516](https://doi.org/10.1021/jacs.9b03516)

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