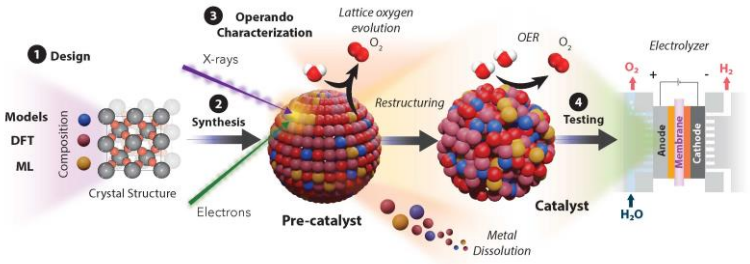
# SCIENCE AT THE ADVANCED PHOTON SOURCE

## USING MACHINE LEARNING TO FIND BETTER ELECTROCHEMICAL CATALYSTS

Hydrogen may be the most common element in the universe, but that doesn't mean it's easy to get when we need it, such as for use as an energy source and storage method. "Green hydrogen," as it's known, is generated by splitting water into its component atoms through electrolysis, but that requires materials for an electrolyzer that can catalyze the reaction, some of which are rare and expensive.

Finding alternative electrocatalysts is therefore an important goal in the quest for a carbon-neutral energy grid. But it's a big job because so many chemical possibilities must be evaluated. Researchers turned to the artificial intelligence technique of machine learning to efficiently screen thousands of possible catalysts and identify some likely choices. Their work appeared in the *Journal of the American Chemical Society*.

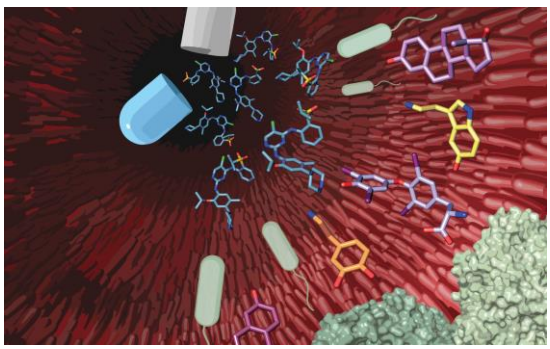
After training a neural network algorithm model on 36,465 metal oxide structures, the investigators substituted 46 elements in the oxide structure while keeping the rutile oxide structure intact. This led to a set of 2070 hypothetical candidates, which were then evaluated for their Pourbaix electrochemical stability. Through this process, the $Ru_{0.6}Cr_{0.2}Ti0.2O_x$ structure was identified as the best possibility. Various experiments and observations, including transmission electron microscopy (TEM), STXM spectroptychography and XANES, were conducted to determine overpotentials, electrochemical performance, stability and morphology of the sample catalysts. The work revealed that the substitution of Cr and Ti in the ruthenium oxide lattice greatly enhances its stability and electrochemical activity.




J. Abed, et. al., "Pourbaix machine learning framework identifies acidic water oxidation catalysts exhibiting suppressed ruthenium dissolution," *J. Am. Chem. Soc.*, 2024, 146, 23, 15740-15750 (June 2024)

The AI-accelerated workflow for catalyst design in this work, starting from design and synthesis, through characterization, and ending with testing the catalyst in a real electrolyzer for hydrogen production.

Aside from identifying a potentially useful OER catalyst for use in PEM electrolyzers, the work demonstrates a computational solution that could be quite valuable not only for discovering further OER electrocatalysts but candidate materials for other electrochemical applications. Scanning transmission X-ray microscopy also proved to be extremely valuable for observing spatial and temporal changes over time, and to map metal-oxygen covalency improvements across the nanoparticle.



J.B. Simpson, et. Al., "Gut microbial ß-glucuronidases influence endobiotic homeostasis and are modulated by diverse therapeutics," *Cell Host and Microbe*, 32, 6, 925-944.e10 (June 2024)

Researchers pinpoint the gut microbial enzymes (green) that reactivate neurotransmitters and hormones (yellow, orange, and purple) essential to homeostasis and to diseases ranging from cancer to anxiety. They also show that a range of FDA-approved drugs (blue) inhibit these enzymes.

## GUT ENZYMES MAY EXPLAIN DIFFERENTIAL DISEASE AND FDA-APPROVED DRUG OUTCOMES

A team of scientists has discovered a new class of enzymes from bacteria in our guts that can alter levels of serotonin, the "feel good" neurotransmitter, and estradiol, a sex hormone, among other compounds. The scientists also found that certain FDA-approved drugs can inhibit these bacterial enzymes. In this way, a cancer drug may inadvertently cause depression in some people by interfering with excretion and thereby initiating a change in their serotonin levels.

Using the Advanced Photon Source, the team collected data that enabled them to solve the crystal structures of various species of gut microbes in complex with various anticancer and antidepressant drugs. What they found not only surprised them but also doubled the pool of enzymes that matter – they'd discovered that a whole other class of enzymes, called C-Terminal Domain GUS (CTD), are critically efficient at processing the sugar-attached molecules and are very potently inhibited by certain drugs.

The findings suggest that off-target responses to drugs may lie in a person's microbiome. For instance, an anticancer drug may cause depression by indirectly dysregulating serotonin levels. It may also explain why some drugs work for some people but not for others. The clinical applications of these findings are clear. When doing a workup and deciding on a treatment regimen, a doctor can now begin to consider a personalized approach, analyzing not only the patient's genome but also the genome of their microbiome.

Read more about the upgraded APS at aps.anl.gov

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