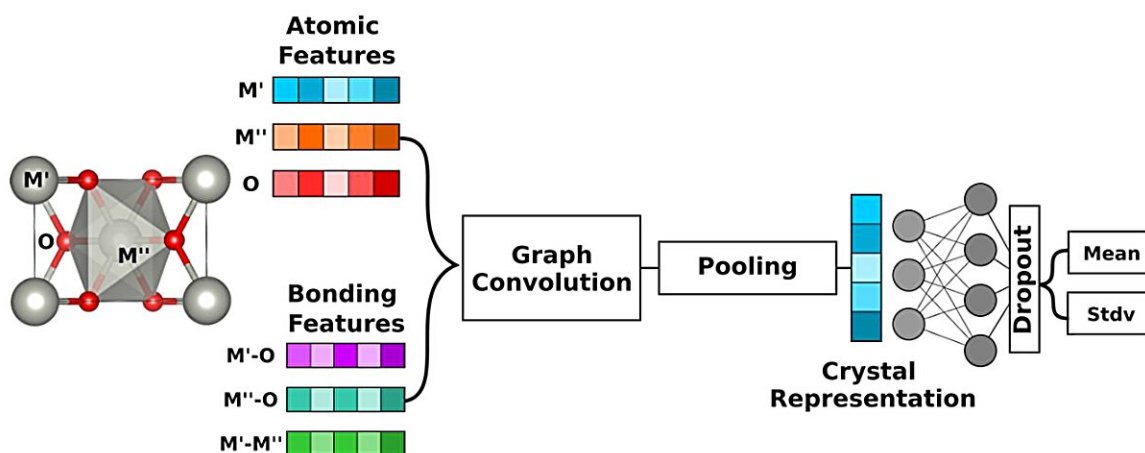# Team using AI finds a cheaper way to make green hydrogen

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CGCNN-HD model architecture. Credit: *Journal of the American Chemical Society* (2024). DOI: 10.1021/jacs.4c01353

Researchers at the University of Toronto are using artificial intelligence to accelerate scientific breakthroughs in the search for sustainable energy. They have used the Canadian Light Source (CLS) at the University of Saskatchewan (USask) to confirm that an AI-generated "recipe" for a new catalyst offered a more efficient way to make hydrogen fuel.

To create green hydrogen, you pass electricity that's been generated from

renewable resources between two pieces of metal in water. This causes oxygen and hydrogen gases to be released. The problem with this process is that it currently requires a lot of electricity and the metals used are rare and expensive.

Researchers are searching for the right alloy, or combination of metals, that would act as a catalyst to make this reaction more efficient and affordable. Traditionally, this search would involve trial and error in the lab, but when you are trying to find the proverbial needle in a haystack, this approach takes too much time.

"We're talking about hundreds of millions or billions of alloy candidates, and one of them could be the right answer," said Jehad Abed. He was part of a team that developed a computer program to significantly speed up this search.

The findings are published in the *Journal of the American Chemical Society*. At the time of this project, Abed was a Ph.D. student under the supervision of Edward Sargent at the University of Toronto working alongside scientists at Carnegie Mellon University.

The AI program the team developed took over 36,000 different metal oxide combinations and ran virtual simulations to assess which combination of ingredients might work the best. Abed then tested the program's top candidate in the lab to see if its predictions were accurate.

The team used the CLS's ultra-bright X-rays to analyze the catalyst's performance during a reaction. "What we needed to do is use that very bright light at the Canadian Light Source to shine it on our material and see how the atomic arrangements would change and respond to the amount of electricity that we put in," said Abed. The researchers also used the Advanced Photon Source at the Argonne National Laboratory in Chicago.

The alloy, a combination of the metals ruthenium, chromium, and titanium in specific proportions, was a clear winner, according to Abed.

"The computer's recommended alloy performed 20 times better than our benchmark metal in terms of stability and durability," he said. "It lasted a long time and worked efficiently."

While the AI program Jehad and colleagues developed shows great promise, the material itself still needs to undergo lots of testing to ensure it will last under "real world" conditions.

"The computer was right about this alloy being more effective and stable. That was a breakthrough because it shows that this method for finding better catalysts is working," said Abed. "What would take a person years to test, the computer can simulate in a matter of days."

The researchers are hopeful that AI will offer a faster route to finding the answers we need to make green energy practical for widespread use.

More information: Jehad Abed et al, Pourbaix Machine Learning Framework Identifies Acidic Water Oxidation Catalysts Exhibiting Suppressed Ruthenium Dissolution, *Journal of the American Chemical Society* (2024). DOI: 10.1021/jacs.4c01353