Scientists break "bottleneck" in hydrogen electrolysis technology

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Clean hydrogen will be crucial to decarbonise the chemical industry. Image BASF

Scientists have made an important discovery that they say "breaks a bottleneck" in the process of extracting hydrogen from water through electrolysis, a discovery that combines the use of machine learning to make water electrolysis more efficient.

The team of scientists, led by Jason Xu Zhichuan, Associate Professor at Nanyang Technological University, Singapore (NTU Singapore), have been studying a class of low-cost hydrogen catalysts called spinel oxides.

Typically made of cheap transition metals, spinel oxides have recently garnered interest as a potentially stable and low-cost hydrogen catalyst that could theoretically reduce energy loss in the electrolytic chemical reaction which extracts hydrogen from water using electricity.

However, the design of high-performing spinel oxides has been restricted due to the fact that there was not much known about how exactly they worked.

Now, the research led by NTU Singapore has made two significant advances which help to shed light on how spinel oxides work. Firstly, they have unravelled, at the atomic scale, how spinel oxides work to speed up water electrolysis. Secondly, the team used machine learning combined with their newfound understanding to select new spinel oxides that increased catalytic activity and, in turn, made water electrolysis more efficient.

"To improve the performance of spinel oxides, we need a deeper understanding of how they work as catalysts to make water electrolysis more efficient," said Associate Professor Xu of the NTU School of Materials Sciences and Engineering.
"Now, by identifying the parameters that make spinel oxides good catalysts for this process, we can create new, better spinel oxides based on these parameters, bringing us one step closer to a hydrogen-powered economy."

The push towards a hydrogen-powered economy has increased over recent years, thanks in large part to the development of more "green hydrogen" projects – hydrogen production projects which are powered by and paired with renewable energy projects such as wind and solar. These 'green hydrogen' projects use the generated renewable electricity to power the electrolysis process, creating a green fuel with little to no emissions involved in the production process.

Beyond the idea of hydrogen being used for passenger and commercial vehicles – especially long-haul commercial vehicles – and as a replacement for traditional aviation fuels, hydrogen could also serve as a viable energy storage alternative to batteries.

One of the roadblocks to the widespread upscale of hydrogen is the bottleneck created in the two primary chemical reactions that take place in the electrolytic process – one, which results in hydrogen production, the other, which leads to oxygen production, the two then are kept separate by a membrane. According to Professor Xu, the bottleneck they sought to break is the chemical reaction that leads to oxygen generation from the other side known as oxygen revolution reaction.

"The oxygen evolution reaction is critical to the efficiency of devices that split water to produce hydrogen fuel, but it is also a sluggish chemical reaction that lowers the overall energy conversion efficiency," Professor Xu explained.

"This is why we need catalysts such as metal oxides to speed things up."

Precious metal oxides have proven to be state-of-the-art electrolytic catalysts, reducing energy consumption and enhancing energy conversion efficiency. However, as with the production of lithium-ion batteries, the scarcity of these precious metals, their high cost and poor durability, have limited their application at a large scale, hamstringing the development of upscaling hydrogen production.

Enter spinel oxides, with their low cost and abundant availability, which present a potential viable alternative to drive down costs and increase efficiency. However, these spinel oxides must be designed with the right parameters, such as the type of transition metal in the spinel oxide, to increase catalytic activity.

The Singapore NTU-led team, with their newfound understanding of spinel oxides, trained a machine learning model with a dataset of over 300 spinel oxides in order to screen and predict the efficiency of any spinel oxide catalyst in a matter of seconds. This method allowed the team to find a new oxide comprising manganese and aluminium which predicted to show superior catalytic activity, a prediction which was validated experimentally.

“While the ability to design highly efficient catalysts greatly pushes forward the technique of water electrolysis in hydrogen production, there are two other major bottlenecks we have to look at before widespread adoption of this technique is possible,” said Professor Xu. “Firstly, we have to improve the membrane in such alkaline electrolysers to support long-term hydrogen production.

“When that’s done, then we can work with our engineering colleagues to see how we can put all of these upgrades into an electrolyser that can function on an industrial level.”