

Running on empty: New affordable catalyst relies on nitrogen vacancies to produce ammonia

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A Low-Cost and Highly Effective Catalyst to Fill Our Ammonia Needs

Ammonia (NH₃)

Pivotal in the fertilizer industry

Hydrogen carrier

However, direct use of N₂ is challenging

Strong bond

Ruthenium

Catalysts for green NH₃ use precious metals

New Ni-loaded LaN catalyst with nitrogen vacancies (V_N)

- 1 Ni nanoparticle dissociates H₂
- 2 H is released and combines with N in lattice to form NH₃
- 3 V_N is formed
- 4 N₂ becomes anchored at V_N (bond weakens)
- 5 Another released H combines with adsorbed N
- 6 NH₃ is formed

New V_N generated by H₂

Highly efficient NH₃ synthesis

As good as state-of-the-art ruthenium catalysts

New design concept for catalysts

Vacancy-enabled N₂ activation for ammonia synthesis on an Ni-loaded catalyst
 Ye et al. (2020) | 10.1038/s41586-020-2464-9
 Nature

東京工業大学
Tokyo Institute of Technology

Nickel-loaded lanthanum nitride (LaN) enables stable and highly efficient ammonia synthesis. Nitrogen vacancies are generated on LaN with low formation energy, and efficiently bind and activate N₂. Credit: Tokyo Tech

Ammonia (NH₃) is one of the most commonly produced chemicals worldwide, because of its use as an important ingredient in a broad range

of industrial manufacturing processes. For instance, it is pivotal in the production of fertilizers, and over 150 million tons of it are applied each year to increase the yields of various crops. Ammonia is produced naturally by many living organisms, but synthesizing it artificially using nitrogen (N_2) and hydrogen (H_2) gasses is challenging because the strong bond between N atoms is difficult to break.

While a method to produce NH_3 at the industrial scale, called the Haber-Bosch process, has existed since the beginning of the 20th century, today's best performing approach involves the use of ruthenium, an expensive and scarce metal, as [catalyst](#) to trigger the necessary reactions. Recently, Prof Hideo Hosono and colleagues from Tokyo Institute of Technology (Tokyo Tech), Japan, have developed a new strategy to produce NH_3 using lanthanum (La), a much more abundant element, in combination with nickel (Ni).

In their paper, published in *Nature*, they explain how they drew inspiration from a previously reported NH_3 production catalyst with the formula Co_3Mo_3N , which bears nitrogen vacancies—locations where the presence of a nitrogen atom would be expected but that are actually empty. These vacancies were observed to make the splitting of N_2 molecules easier, which led Hosono's team down a new direction of exploration for more readily available and effective NH_3 synthesis catalysts. He explains: "The critical role of the nitrogen vacancies in Co_3Mo_3N inspired us to consider other nitrogen-containing materials on which vacancies could be generated easily as the basis for new Ni-based catalysts."

The catalyst they developed consists of LaN crystals loaded with Ni nanoparticles. The Ni easily dissociates H_2 into H atoms. Thus, pre-treatment of the catalyst with H_2 readily generates H atoms, which then react with the N [atoms](#) in the [crystal structure](#) to form NH_3 and create N vacancies on the LaN support. Each of these empty sites then captures

an N atom from an N_2 molecule from the input nitrogen gas, causing the molecule's N-N bond to weaken. Another dissociated H atom breaks the weakened N-N bond to produce more NH_3 , leaving an N atom behind to fill the original vacancy. These cycles repeat themselves, thereby continuously generating [nitrogen](#) vacancies and sustaining the synthesis process.

This concept of a "dual active site" catalyst turned out to be very promising. The proposed catalyst's performance far exceeds that of more conventional cobalt- and nickel-based catalysts and is comparable to even that of ruthenium-based ones: It not only consistently produces high yields of ammonia at moderate temperature and pressure, its structure is maintained even after 100 hours of continuous reaction, demonstrating its high stability.

Hosono says, "We anticipate that our work will stimulate further exploration of catalyst designs that make use of more abundant elements. In particular, our results illustrate the potential of using vacancy sites in reaction cycles and point to a new design concept for catalysts for ammonia synthesis."

The new strategy could make the production of ammonia simpler and more affordable, thus easing a multitude of significant industrial processes.

More information: Vacancy-enabled N_2 activation for ammonia synthesis on an Ni-loaded catalyst, *Nature* (2020). [DOI: 10.1038/s41586-020-2464-9](https://doi.org/10.1038/s41586-020-2464-9)

Provided by Tokyo Institute of Technology

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