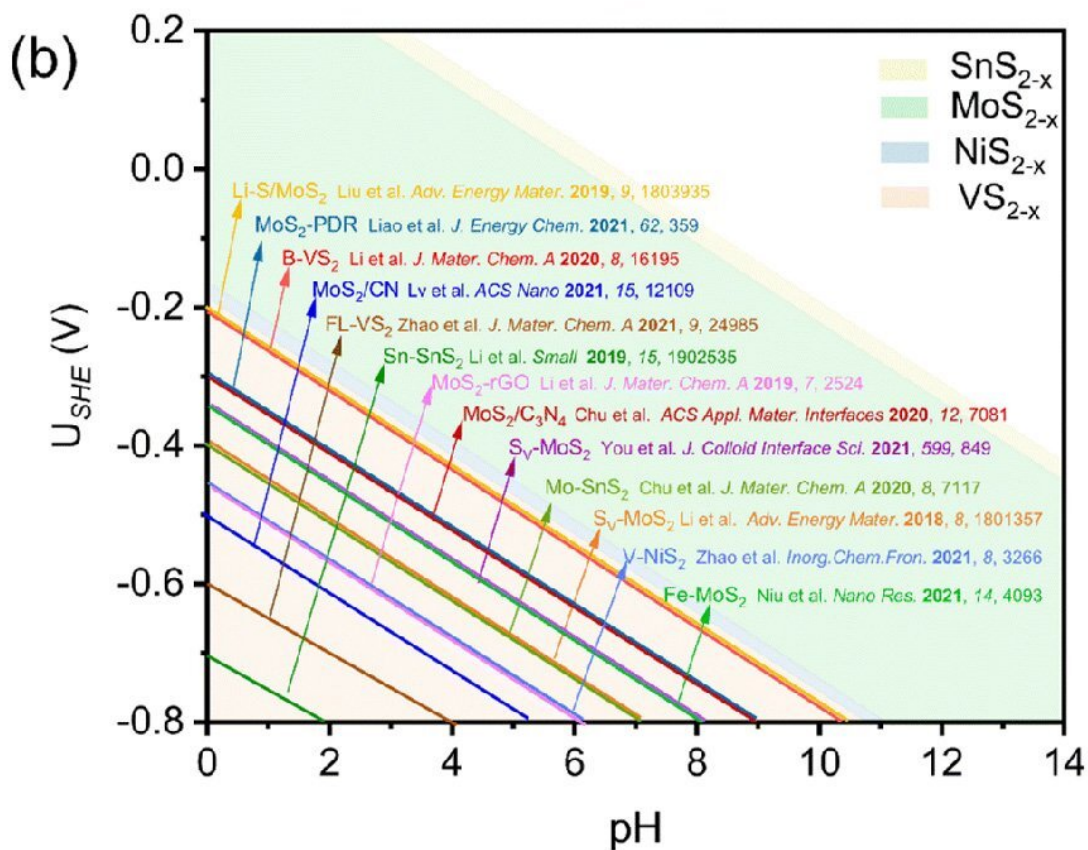
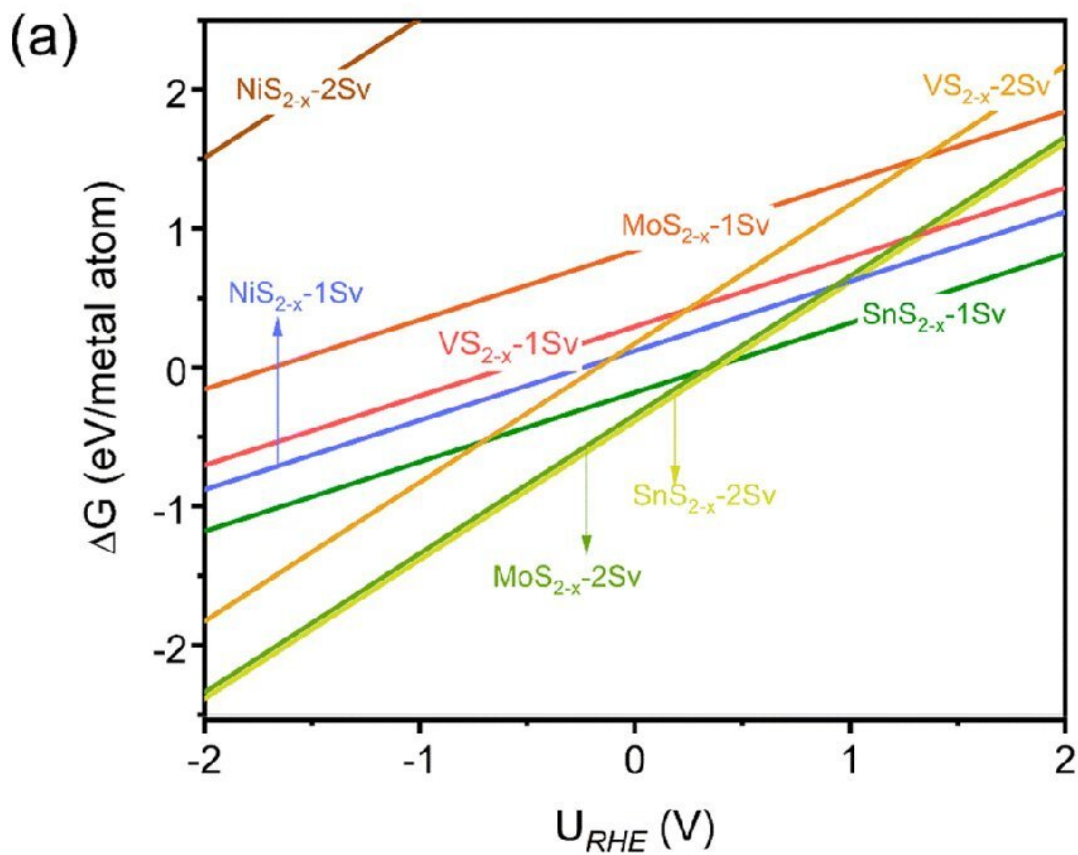


Researchers propose electrocatalytic ammonia synthesis as a more environmentally friendly method

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(a) 1D surface Pourbaix diagrams of different transition metal disulfide (TMS_2) surfaces. (b) 2D surface Pourbaix diagram of S_V formation as a function of pH and potential. The color-coded segments demarcate the potential windows of S_V generation on the respective instances of TMS_2 . Credit: *Journal of Materials Chemistry A* (2024). DOI: 10.1039/D4TA00307A

A team of researchers has unveiled a promising alternative to the conventional means of synthesizing ammonia, one that is more environmentally friendly.

Details of their research were [published](#) in the *Journal of Materials Chemistry A* on February 21, 2024.

When Fritz Haber and Carl Bosch invented a means to synthesize ammonia from nitrogen and hydrogen gas in the early 20th century, it enabled the production of the chemical at an industrial level. To this day, the Haber-Bosch synthesis remains the dominant means of producing ammonia.

Yet the method has some environmental drawbacks. It is energy and resource intensive, and producing [hydrogen gas](#) often involves natural gas, which releases carbon dioxide as a by-product.

The electrochemical nitrogen reduction reaction (ENRR), where nitrogen gas from the air can be converted into ammonia using an [electrical current](#), is seen as a promising and sustainable alternative. Pursuing high-performance and cost-effective ENRR catalysts, however, is an open challenge for achieving commercial-scale ambient ammonia production.

"We explored the potential of less-precious transition metal disulfides (TMS_2) as catalysts for ENRR," says Hao Li, associate professor at Tohoku University's Advanced Institute for Materials Research (WPI-AIMR) and corresponding author of the paper. "Through meticulous analysis of electrochemistry-induced surface states, we uncovered a previously unrecognized factor contributing to their high ENRR performance: S-vacancy generation."

Li and his colleagues started with a typical ENRR TMS_2 catalyst, iron disulfide (FeS_2), where they observed that under ENRR conditions, S-vacancies can be easily generated on the [catalyst](#) surface. Through advanced computational simulations, they demonstrated that this electrochemistry-driven "in situ" generation of S-vacancies significantly enhances ENRR activity by promoting stronger N–N adsorption and activation.

Experimental observations confirmed their findings, which were also consistent with recent literature on ENRR potential windows reaching maximum Faradaic efficiency—the measure of the effectiveness of an electrochemical process in converting electrical energy into [chemical energy](#) or vice versa.

Their analysis also extended to other TMS_2 catalysts (SnS_2 , MoS_2 , NiS_2 , and VS_2), revealing a universal phenomenon of "in situ" S-vacancy generation under ENRR potentials.

"Our research underscores the critical importance of considering surface states in the design of ENRR catalysts," adds Li. "By shedding light on the role of S-vacancies, we have provided a valuable roadmap for enhancing ENRR performance and accelerating the transition towards sustainable [ammonia](#) production."

More information: Tianyi Wang et al, Origin of electrocatalytic nitrogen reduction activity over transition metal disulfides: critical role of in situ generation of S vacancy, *Journal of Materials Chemistry A* (2024). [DOI: 10.1039/D4TA00307A](https://doi.org/10.1039/D4TA00307A)

Provided by Tohoku University

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