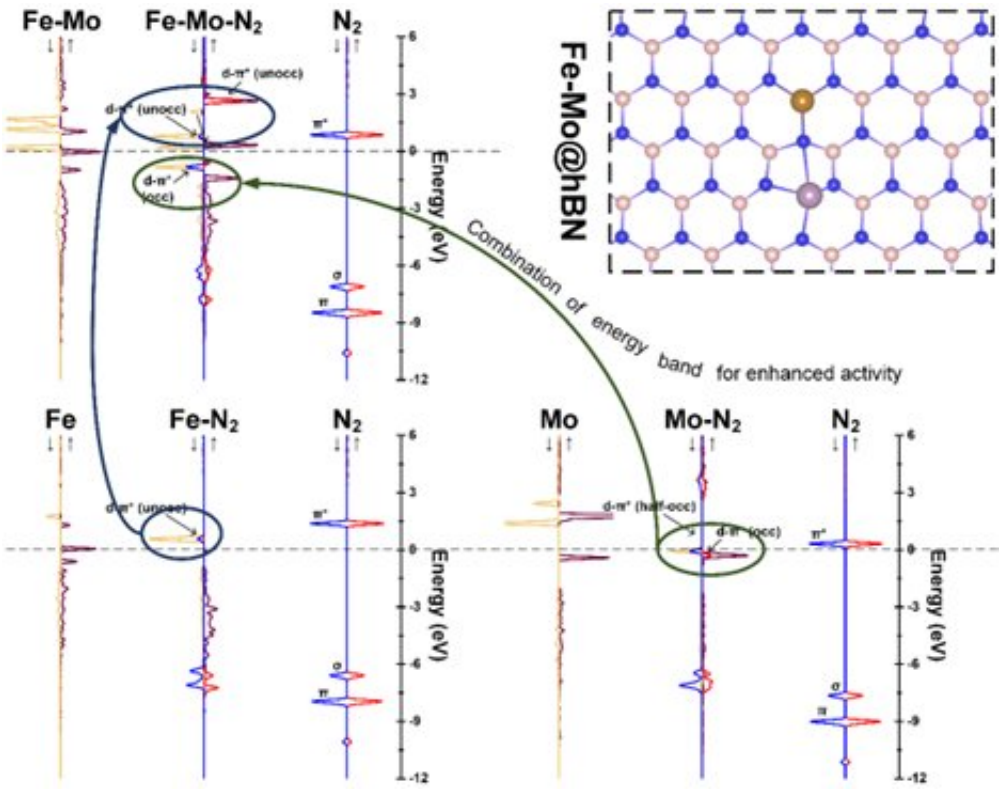
Novel design for dual-atom catalyst could reduce the environmental impact of ammonia production

August 5 2022



How the heterogeneous catalyst integrates properties of the components to enhance catalytic performance. Credit: Southeast University, China

Ammonia is a strong-smelling, colorless gas that has become an essential chemical for agriculture and pharmaceutical companies, with around 200 million tons produced and consumed each year.

The Haber-Bosch process is the only option currently available for industrial production of ammonia, but the elevated temperature and pressure it requires, leads to high energy use and CO_2 emission rates. As a result, researchers have been seeking new energy-saving and eco-friendly methods for ammonia synthesis. The electrocatalytic reduction of dinitrogen, a colorless, odorless gas that makes up approximately 78% of the Earth's atmosphere, is proving a promising approach.

In a study published in the KeAi journal *Green Energy & Environment*, researchers screened dozens of single-atom and double-atom catalysts in a bid to find a new, more green option for the dinitrogen reduction process. Study author Qiang Zhou, who is currently a Ph.D. student in the Department of Mechanical Engineering at Japan's Tokyo University, explains: "Catalyst design is the most crucial element in successful electrocatalytic dinitrogen reduction. We knew that heterogenous catalysts, in other words, catalysts with multiple phases, have the highest ammonia yield rate, but we wanted to find out why, and then use that knowledge to identify new, even more effective electrocatalytic options."

Zhou and his colleagues used density functional theory (DFT), a computational quantum mechanical modeling method used to investigate the electronic structure of systems, such as atoms and molecules. According to Zhou, "it is widely employed to design novel catalysts, to support experimental results, and to investigate catalytic mechanism. We knew that DFT simulation would not only help us know which catalysts worked well, but know why they worked well. And that would help us better understand the reaction process and design better catalysts."

Using DFT computation, the research team systematically screened and compared dozens of single-atom catalysts. This gave them vital information to develop a general strategy for the design of dual-atom (heterogeneous) catalysts. They found that a dual-atom approach using a

hybrid of iron and molybdenum was the most effective at activating the dinitrogen.

According to Dr. Feng Gong, an investigator from Southeast University, China, who led the study, this finding has the potential to greatly impact the field of heterogeneous catalysis. He adds: "It is our hope it will provide some guidelines for future experimental synthesis of dual-atom catalysts and encourage scientists to continue exploring the mechanism of catalytic reactions."

More information: Qiang Zhou et al, 1+1>2: Learning from the interfacial modulation on single-atom electrocatalysts to design dual-atom electrocatalysts for dinitrogen reduction, *Green Energy & Environment* (2022). DOI: 10.1016/j.gee.2022.06.005

Provided by KeAi Communications Co.