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Minkee Choi began his academic training in chemistry at the Korea Advanced Institute of Science and Technology (KAIST), where he received his B.S. in 2002. He remained at KAIST for graduate studies under the guidance of Prof. Ryong Ryoo, earning his M.S. in 2004 and Ph.D. in 2007. After completing his doctorate, he continued at KAIST as a postdoctoral researcher until 2009, before joining the Department of Chemical Engineering at the University of California, Berkeley, for a postdoctoral appointment with Prof. Enrique Iglesia. In late 2010, he returned to KAIST as an Assistant Professor in the Department of Chemical and Biomolecular Engineering. He was promoted to Associate Professor in 2015 and is currently serving as a Full Professor.

Choi's research centers on the design and application of functional porous materials, including zeolites, silica, alumina, polymers, carbons, and their composites. His work spans catalytic and adsorption processes, with a particular interest in molecular diffusion and acid site distributions in zeolites, as well as interfacial control in supported metal catalysts. His group also investigates advanced materials for environmental applications such as water treatment and post-combustion CO_2 capture.

His scientific contributions have been recognized with several honors, including the Distinguished Lectureship Award from the Chemical Society of Japan (2014), and the Minister's Award in Invention Day (2019). He was elected to the Young Korean Academy of Science and Technology (Y-KAST) in 2019. Further recognition includes the Young Scientist Award from the President of the Republic of Korea (2021), the Young Catalysis Researcher Award from the Korean Institute of Chemical Engineers (2022), and the 2024 SCEJ Award for Outstanding Asian Researcher and Engineer from the Society of Chemical Engineers, Japan. He currently serves on the Editorial Advisory Board of ACS Catalysis.

Separately Storing Electrons and Protons at Ru Particles and Base Promoters to Facilitate Ammonia Synthesis

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Ammonia (NH_3) is crucial for the production of fertilizers, pharmaceuticals, and explosives, and it has attracted great attention as a carbon-free fuel and hydrogen carrier. Recently, there has been a strong demand for catalysts that enable ammonia synthesis under mild conditions (<573 K, <2 MPa) to efficiently integrate with electrolytic H_2 production. The main challenge of NH_3 synthesis under such conditions lies in activating the stable N≡N bonds of N_2, which necessitates the development of more advanced catalysts. Ru catalysts combined with base promoters (e.g., Ba, Cs, La oxides) have shown promising NH_3 synthesis activities under mild conditions. However, even the most recent catalysts suffer from insufficient activities and significant H_2 poisoning. Furthermore, a comprehensive understanding of the promoting mechanism and the structure-property correlation of the catalysts is still lacking.

In this study, we carried out rigorous analysis of 24 catalysts (22 carbon-supported and 2 MgO-supported Ru catalysts) during NH_3 synthesis under mild conditions (573 K and 10 bar). An extremely wide range of NH_3 production rates (0.9–342.3 mmol g_{Ru}^{-1} h^{-1}) was observed, depending on the types of supports and BaO promotion. This variation is striking, considering that all catalysts have similar Ru dispersions and loadings. A complementary combination of spectroscopic analyses indicated that H atoms generated by H_2 activation on Ru dissociate into H^+/e^- pairs. Subsequently, H^+ migrates over the carbon surfaces to titrate remotely placed basic BaO, while e^- accumulates in conductive Ru/carbon bodies (Fig. 1). Conversely, on the surface of the insulating MgO support, H splitting into H^+/e^- occurs only at the intimate BaO–Ru interfaces. As the work function of the carbon support decreases relative to that of Ru (4.67 eV), e^- is gradually localized in Ru particles in Ba-Ru/carbon catalysts, facilitating N_2 activation via π-backdonation and alleviating H_2 poisoning. Consequently, the work function of the carbon support turns out to be the most critical descriptor for the NH_3 production rates of the Ba-Ru/carbon catalysts. The best catalyst, synthesized using low-work-function N-doped multiwalled carbon nanotubes, exhibited 7.4 times higher activity than Ba-Ru/MgO, a benchmark catalyst.

Our results clearly demonstrate that Ru and BaO domains, connected by conductive low-work-function carbon supports, can store e^- and H^+ separately under the reductive reaction conditions, leading to very high NH_3 synthesis activities. These catalysts can be considered 'chemical capacitors' because they store two differently charged species, electrons (e^-) and H^+ ions, through the chemical action of BaO (a strong base). The electronic promotion effects of BaO, well-recognized in the literature for a long time, appear not to stem from simple inductive effects, but rather from such charge capacitive effects.

This study provides crucial atomistic insights into the role of base promoters and offers significant perspectives for designing advanced NH_3 synthesis catalysts. The results showed that charge distribution within catalysts can be significantly altered under reaction conditions, and its rational control can enable the design of active NH_3 synthesis catalysts. Specifically, we believe that the development of new nanostructured carbon supports with lower work functions and higher crystallinity holds promise for creating highly active and stable Ru catalysts for NH_3 synthesis.

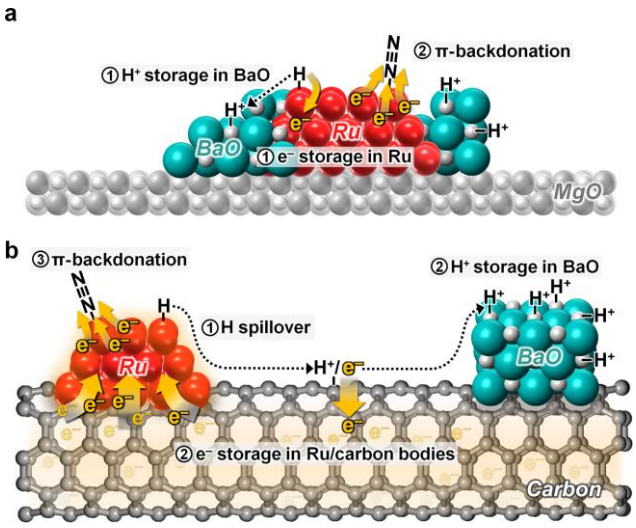

Fig. 1. Hydrogen-aided electron donation of BaO to Ru during NH_3 synthesis. a, BaO-promoted Ru catalysts on an insulating MgO support. Chemisorbed H atoms on Ru polarize into H^+/e^- pairs at the BaO–Ru interfaces, where nonreducible BaO selectively captures H^+ while leaving e^- in Ru. b, BaO-promoted Ru catalysts on a conductive carbon support. H^+/e^- pairs can migrate over long-distances across the carbon surface. BaO can capture H^+ even without direct contact with Ru, while accumulating e^- in the conductive Ru/carbon bodies.

References

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