## [Grant-in-Aid for Scientific Research (S)]

# **Broad Section D**



Title of Project: Low temperature ammonia synthesis by heterogeneous catalysts enhancing electron-donating power

Michikazu Hara (Tokyo Institute of Technology, Institute of Innovative Research, Professor)

Research Project Number: 18H05251 Researcher Number: 70272713

Keyword: Heterogeneous catalyst, Ammonia synthesis

### [Purpose and Background of the Research]

The mass production of ammonia by so-called "Haber-Bosh process" using iron-based catalysts has supported the increase in human population and modern civilization for over 100 years. Because ammonia synthetic reaction is an exothermic increase in reaction temperature immediately decreases ammonia yield. In fact, the maximum ammonia yield at 400 °C cannot transcend 40% even under a high pressure of 20 MPa. For this reason, commercial ammonia production process using iron-based catalysts with high working temperatures over 400 °C requires compression to tens-a few tens MPa in order to achieve an ammonia yield of ca. 30%, causing large energy consumption and heavy manufacturing plant. Thus, further decrease in catalyst working temperature for increase in ammonia yield has been remaining as a challenging subject since ammonia production by Haber-Bosch process.

The aim of this study is to create a new heterogeneous catalytic system to give an ammonia yield over 80% under pressures below 5 MPa, i.e. a novel heterogeneous catalyst that works efficiently for ammonia synthesis below 150 °C, to overcome the above drawback in conventional ammonia production.

#### [Research Methods]

In this study, the desired catalyst is created by combining transition metal nanoparticles as active sites with a family of strong electron-donating materials that have both low work functions and stability under ammonia synthetic conditions via the followings.

- 1. The optimal combination of transition metal nanoparticles with the strong electron-donating materials as supports is found by examining ammonia synthetic activities for transition metal nanoparticles-deposited electron-donating materials.
- 2. The electron-donating capability of the selected electron-donating material is remarkably enhanced though several methods.
- 3. The catalyst consisting of transition metal nanoparticles and support enhancing electron-donating capability is examined through

ammonia synthesis below 150 °C and 5 MPa to find the working principles for further efficient catalysts.

# [Expected Research Achievements and Scientific Significance]

While "Wind to Ammonia" (Figure 1), on-site ammonia production using  $H_2$  form wind power station, is attracting public attention as a sustainable ammonia production without using fossil resources, this is difficult to realize because conventional Haber-Bosch process consumes too much energy. This study to decrease energy consumption for ammonia synthesis can enable sustainable ammonia production through "Wind to Ammonia".



Figure 1 Wind to ammonia

## [Publications Relevant to the Project]

- Komanoya, T; Kinemura, T; Kita, Y; Kamata, K; <u>Hara, M</u>\*, "Electronic Effect of Ruthenium Nanoparticles on Efficient Reductive Amination of Carbonyl Compounds", *J. Am. Chem. Soc.*, **139**, 11493–11499, 2017.
- <u>Hara, M</u>\*; Kitano, M; Hosono, H\*, "Ru-Loaded C12A7:e Electride as a Catalyst for Ammonia Synthesis", *ACS Catalysis*, 7, 2312-2324, 2017.

[Term of Project] FY2018-2022

**(Budget Allocation)** 146,600 Thousand Yen

# [Homepage Address and Other Contact Information]

http://www.msl.titech.ac.jp/~hara mhara@mas.titech.ac.jp.