【Grant-in-Aid for Scientific Research (S)】

Broad Section E

Title of Project： Development of Innovative Molecular Transformations from Molecular Dinitrogen Using Super-Catalysts

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Research Project Number: 20H05671 Researcher Number：40282579
Keyword：molecular dinitrogen, ammonia, catalyst

【Purpose and Background of the Research】

The principal investigators have recently developed a highly efficient method for the catalytic synthesis of ammonia from nitrogen gas using water as a proton source under extremely mild reaction conditions at ambient temperature and pressure. Based on the research results achieved so far, the main objective of this project is to gain insight into the fundamental technologies for the development of 'super-catalysts' beyond the previously developed series of catalysts and their use to achieve innovative molecular transformations of molecular nitrogen with very low reactivity.

In parallel with the main objective, there is a need to develop a new aspect of ammonia utilization, namely, the use of ammonia as an energy carrier, and we have very recently succeeded in developing a method for extracting energy from ammonia. Based on the research results achieved so far, we will also work to gain knowledge on fundamental technologies to achieve the development of "super-catalysts" that surpass the series of catalysts we have developed so far and to develop ammonia decomposition reactions using them.

【Research Methods】

(1) Development of ammonia synthesis methods

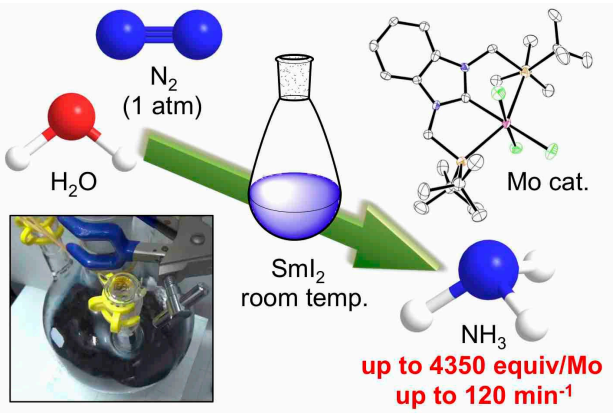
The principal investigator and co-workers have already shown that molybdenum complexes with PCP-type pincer ligands containing carbene skeletons work as effective catalysts for the catalytic ammonia synthesis. In order to gain a detailed insight into the catalytic reaction, DFT calculations are performed for all steps of the catalytic reaction, as well as isolation of key intermediates formed during the catalytic reaction and their stoichiometric and catalytic reactivities. We will attempt to develop new molecular catalysts for more efficient ammonia synthesis by feeding back the findings of the series of investigations into catalyst design.

(2) Development of ammonia decomposition methods

The principal investigator and co-workers have already shown that ruthenium complexes with bipyridine ligands work as effective catalysts for catalytic ammonia decomposition reactions. In order to gain a detailed insight into the catalytic reaction, DFT calculations are performed for all stages of the reaction, as well as isolation of key intermediates formed during the catalytic reaction and their stoichiometric and catalytic reactivities. The findings from the series of investigations will be fed back to the design of the catalysts in an attempt to develop new molecular catalysts for more efficient ammonia decomposition.

【Expected Research Achievements and Scientific Significance】

Results of this research are expected to make a major breakthrough directly in related research fields such as coordination chemistry and catalytic chemistry, as well as having a major impact on a wide range of related research fields such as organic chemistry and organometallic chemistry. The development of a next-generation ammonia synthesis method will not only be an academic achievement, but also a groundbreaking industrial breakthrough, and will be an achievement that will go down in history.



【Publications Relevant to the Project】

- Molybdenum-Catalysed Ammonia Production with Samarium Diiodide and Alcohols or Water, Y. Ashida, K. Arashiba, K. Nakajima, Y. Nishibayashi, *Nature*, **2019**, *568*, 536-540.
- Ruthenium-Catalysed Oxidative Conversion of Ammonia into Dinitrogen, K. Nakajima, H. Toda, K. Sakata, Y. Nishibayashi, *Nature Chemistry*, **2019**, *11*, 702-709.

【Term of Project】 FY2020-2024

【Budget Allocation】 153,600 Thousand Yen

【Homepage Address and Other Contact Information】

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