Usage Report for Fiscal Year 2024

**Project Title:**

# First-principles study of catalytic electrochemical reaction for fuel cell and ammonia synthesis based on hydride ion conduction

**Name:**
**○Shibghatullah MUHAMMADY**

**Laboratory at RIKEN:**
**Solid State Chemistry Laboratory, RIKEN Cluster for Pioneering Research**

## 1. Background and purpose of the project, relationship of the project with other projects

Ammonia is excellent for hydrogen storage due to its high density of hydrogen per mol ammonia. From this storage, hydrogen production and ammonia fuel cells can be utilized for alternative energy applications. However, effective catalyst materials are essential to acquire optimum ammonia synthesis. Here, (1) we aim to analyze the catalysis efficiency of ammonia synthesis on ruthenium surface by employing DFT calculations. Furthermore, (2) we also analyze various properties of hydrides as candidates for ammonia synthesis.

## 2. Specific usage status of the system and calculation method

We used the Hokusai supercomputer facilities to (1) calculate the free energy diagrams of ammonia synthesis on terrace and stepped ruthenium surfaces. Also, we used the facilities to (2) simulate structural, thermodynamics, and electronic properties of defective hydrides.

## 3. Result

From the first part of our research, (1) the thermodynamics analysis shows the deeper free energy diagram during hydrogen adsorption on the stepped surface with lower activation energy of nitrogen dissociative adsorption, leading to more efficient catalysis. In the second part, (2) the hydrogen content increment improves the conductivity but decrease the formation stability. Overall, our result can be used as references for explaining existing experimental results or predicting influences of the modifications of experimental parameters.

## 4. Conclusion

(1) The stepped ruthenium surface is more efficient for ammonia synthesis than the terrace surface. (2) Furthermore, our analysis shows significant influence of hydride concentrations on the thermodynamics and electronic properties.

## 5. Schedule and prospect for the future

This project will be continued in the next fiscal year for employing diffusion of $N_2$ in solid state systems.

## 6. If no job was executed, specify the reason.

## Fiscal Year 2024 List of Publications Resulting from the Use of the supercomputer

### [Paper accepted by a journal]

None

### [Conference Proceedings]

None

### [Oral presentation]

None

### [Poster presentation]

None

### [Others (Book, Press release, etc.)]

None