

# Report for MERIT Internship

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6<sup>th</sup> term MERIT student

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Company name of internship	Nissan Arc Co., Ltd.
Training Department	Device Analysis unit
Training period	September 2 <sup>th</sup> , 2019~October 31 <sup>th</sup> , 2019
Implementation theme	"Characteristic extraction in stable atom arrangement on binary alloy surface"

## Purpose

I set the following three goals for this internship.

- I want to be able to fill the gap between experiment and theory by understanding not only experiments but also theory to some extent.
- I want to experience the life of corporate researchers.
- I want to challenge new things in terms of my own growth. Therefore, I would like to broaden my research field by starting theoretical calculation and machine learning.

In this two-month internship, I was able to learn calculations practically, and the results were very fruitful.

## Background

In recent years, "ENE-FARM" and polymer electrolyte fuel cells used as a power source for fuel cell vehicles use an alloy having a high catalytic function at both the positive electrode and the negative electrode. Alloys are often used for these catalytic reactions, but in reality, structural changes due to defects and dissolution phenomena occur during catalytic reactions, so we should investigate whether stable structures different from the basis can be predicted from calculations. This is considered very important.

## Contents

The most stable structure of binary alloys was searched using machine learning and DFT calculation. As my research was an experimental, and the theoretical one was on the outside, most of them were my first experience. What I particularly worked on was learning machine learning using Python and learning DFT calculations. Neither can be said to have been fully mastered, but I think that I have learned the enough basics to study by myself. The final result was not completely satisfactory, but I think that it has been completed to some extent within the limit of two months. I felt that the internship period of two months was very short because the work ended just after getting on track.

Also, as I was actually surprised that Nissan Ark's work is not only on application but also on basic research. Unfortunately, I heard that the research span at the company was too short, but my internship ended sooner than expected so I didn't feel the time span. Since it was an internship, it was not something related to me but the flextime system was introduced at Nissan Ark, and I felt that there was a degree of freedom in lifestyle. In addition, I felt that international colors were also rich and very diverse. As for the location of the company, the nearest station is along the Keikyu line called Oppama between Yokohama and Yokosuka. There was a direct bus to the company and I was very surprised by it.

Executive officers also attended the report meeting on the last day and gave me compliments about the contents of the report and my response to questions and answers. In this internship, I had little opportunity to use the knowledge I have cultivated so far, but the basics I learned at graduate school, such as thinking about things logically and making research paths, was helpful. Also, since it is a company, I could practice practically how to make my research understood easily for non-specialists.

## Acknowledgement

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