MERIT Internship Program (Domestic) Report

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【 Date 】

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【 Host institute 】

Research Center for Computational Design of Advanced Functional Materials (CD-FMat),
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【 Outline 】

I visited Dr. Takashi Miyake's group in CD-FMat in AIST, which is located in Tsukuba City, Ibaraki Prefecture. The group develops computational methods in solid state physics based on *ab initio* calculations and machine learning frameworks. By using such methods, I investigated magnetic properties of transition metal compounds during the internship.

【 Research 】

As magnetic materials play a key role in various electric devices such as motors and storages, it is highly desired to enable the accurate prediction of their magnetic properties, e.g., the saturation magnetization and the Curie temperature, based on solid state physics. However, it is a difficult challenge as the magnetic materials consist of many correlated electrons. For many decades, previous insightful works have revealed rules of magnetic properties of specific materials from qualitative discussions; the typical example is Goodenough-Kanamori rule, which roughly predicts superexchange interactions in the transition metal compounds from the crystal structures and the number of *d* electrons. Furthermore, the recent development of computer hardware and computational algorithms enables us to investigate the magnetic properties by *ab initio* calculations and analyze big experimental and calculation data by machine learning frameworks. Therefore, the motivation of this study is, based on these computational methods, to revisit the rules of magnetic materials and to expand the rules to more generic forms.

During the internship, I learned computational methods to estimate magnetic interactions from *ab initio* calculations and to analyze calculation data by machine learning frameworks. I applied these methods to the several perovskite-type compounds and studied the systematic behavior of their magnetic interactions. In the future, I will investigate other materials and try to build a computing system to predict magnetic interactions of the transition metal compounds from little essential input, e.g., the crystal structure and constituent elements.

【 Acknowledgement 】

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