

論文 / 著書情報
Article / Book Information

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Category(English)	Doctoral Thesis
種別(和文)	論文要旨
Type(English)	Summary

(博士課程)
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論文要旨

THESIS SUMMARY

系・コース： Department of Graduate major in	材料 材料	系 コース	申請学位 (専攻分野)： 博士 Academic Degree Requested Doctor of	(理学)
学生氏名： Student's Name	SEO Insung		審査員主査： Chief Examiner	合田 義弘

要旨 (英文 800 語程度)

Thesis Summary (approx.800 English Words)

In this dissertation, we explored magnetic properties of rare-earth permanent magnet compounds through first-principles calculations.

In Chapter 1, we explained the importance of permanent magnets and previous research. Due to global environmental issues and the energy crisis, the demand for high-performance permanent magnets is increasing, and many studies are being conducted. However, permanent magnet compounds that surpass Nd₂Fe₁₄B, which was introduced in 1984, have not yet been commercialized. Therefore, we decided to explore and design new permanent magnet materials, using a materials informatics approach that combines materials databases, first-principles calculations, and machine learning. Finally, we introduced our research objectives and the outline of this thesis.

In Chapter 2, we described the main methodologies used in this thesis. First, we introduced the density functional theory used for first-principles calculations and the open-core approximation method for treating rare-earth elements. Second, we briefly listed the calculation methods for important physical properties of magnetic materials, such as formation energy, saturation magnetization, magnetic anisotropy energy, and Curie temperature. Finally, we explained the materials informatics approach and the random forest method, which is the machine learning method we used, and introduced the calculation conditions used in this thesis.

In Chapter 3, we applied the materials informatics approach to the exploration of permanent magnet materials. First, we designed new Nd-Fe-based permanent magnet compounds using simple screening conditions on the crystal structures included in the materials database. During this process, we confirmed that existing magnetic materials such as 1-5, 1-12, and 2-17 structures were included, successfully validating the effectiveness of the approach. Among the compounds discovered using this method, we investigated in detail the most promising candidate for a new permanent magnet compound with the highest saturation magnetization, NdFe₁₆. We calculated the electronic structure of NdFe₁₆, NdFe₁₆X₃ with light elements inserted into the crystal structure. As a result, we observed changes in the electronic structure due to the insertion of light elements and the resulting changes in magnetic properties. Using the data obtained thus far, we started machine learning. We designed descriptors for machine learning and confirmed the effectiveness of the methodology through machine learning. Finally, we included the results of a follow-up study, which discovered new magnetic materials using this methodology.

In Chapter 4, we investigated changes in magnetocrystalline anisotropy energy due to the insertion of light elements using the representative permanent-magnet compounds, 1-12 and 2-17 compounds. We elucidated the complex trends and changes in magnetocrystalline anisotropy energy through electronic structure calculations. We also proposed a methodology to analytically determine the direction of magnetic anisotropy using only the crystal structure without performing electronic structure calculations. This method was not effective for complex ternary systems due to its overly simple assumptions but showed good applicability to R-Fe binary compounds.

Lastly, in Chapter 5, we concluded the dissertation and propose future works.

備考：論文要旨は、和文 2000 字と英文 300 語を 1 部ずつ提出するか、もしくは英文 800 語を 1 部提出してください。

Note：Thesis Summary should be submitted in either a copy of 2000 Japanese Characters and 300 Words (English) or 1copy of 800 Words (English).

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