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Contents

Abstract

In this dissertation, we focus on the exploration of novel magnetic compounds utilizing materials databases and the evaluation of their magnetic properties through first-principles calculations.

In Chapter 1, we introduce the necessity for discovering new rare-earth magnetic compounds suitable as primary phases in permanent magnet materials. We highlights the limitations of previous exploration methods, which have been largely confined to the vicinity of existing magnetic compounds in the materials searching space. This underscores the need for a more expansive exploration. Furthermore, we addresses the current insufficient fundamental understanding of magnetocrystalline anisotropy energy in rare-earth magnetic compounds, which impedes the design of materials with high magnetocrystalline anisotropy energy.

In Chapter 2, we describe the theoretical framework employed in this research. We briefly introduces first-principles electronic theory and theoretical methods for evaluating the stability and magnetic properties of rare-earth magnetic compounds. Additionally, we outlines the machine learning techniques used for compound exploration. Finally, we describes a method for determining interstitial sites of light elements and specifies the computational conditions utilized in this dissertation.

In Chapter 3, we examine numerous potential magnetic compounds by substituting crystal structures of non-magnetic materials from materials databases with Nd-Fe systems. We focus on the $NdFe_{16}$ (1-16) compound, which exhibits saturation magnetization surpassing that of existing magnetic compounds. While the binary 1-16 system lacks sufficient stability, the addition of light elements is shown to reduce formation energy and enhance compound stability. Notably, oxygen addition to 1-16 maintains excellent magnetic properties while lowering formation energy. Based on first-principles calculations of multiple compounds, including 1-16, machine learning using the Random Forest method was employed to screen materials from other databases without substitution. This approach enabled the construction of a database for R-Fe binary compounds, screening over 20,000 materials with significantly reduced computational costs.

In Chapter 4, we aim to enhance the understanding of magnetocrystalline anisotropy energy by focusing on its changes in 1-12 and 2-17 systems upon light element addition. The results reveal non-monotonic, strong variations in magnetocrystalline anisotropy energy with different light element addition. These changes are attributed not only to energy shifts in the $2p$ orbitals due to electronegativity variations but also to orbital hybridization effects inducing alterations in the rare-earth element's electronic configuration. Based on these findings, a framework is proposed to easily predict the direction

of anisotropy energy in R-Fe binary systems solely from atomic arrangements.

Chapter 5 summarizes the dissertation and discusses future prospects.