Machine learning-based prediction of magnetic properties for half-Heusler compounds using atomic information

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September 15, 2021

Abstract

In this paper, we aim to demonstrate the high reliability of the machine learning model for the sought-after parameters. By the end of this paper, we achieved our aim by deploying the atomic information of constituent elements like atomic radii and atomic mass to predict magnetic moment and elasticity. With a little hassle, the ML model trained on the half-Heusler compounds can easily incorporate the full-Heusler compounds. With that in mind, the study is carried out on the half-Heusler compounds. Amongst the two employed ML model, the GBT reported co-efficient of determination to be as high as 0.957. The next model, artificial neural network, was close but stuck around 0.948. Our results may serve as a motivation to harness the robust ML models into the calculation of desired parameters. Which may lead to a low-cost and short-time development of new functional devices and materials.

1 Introduction

A general understanding of how microscopic structures and characteristics gives forth the material properties, which are a necessary prerequisite for designing the next iteration of desired materials. Due to the myriad of applicability, the Heusler alloys receive tremendous experimental and theoretical interest. We are particularly interested in its use for spintronics and as a material. For the same, the calculation of total molecular magnetic moment and elasticity of the compound is the crucial physical parameters. By and large, for this effort, the typical computational simulations like DFT and molecular dynamics are vital tools. So far the Heusler compounds are treated in the equal footing [14, 21]. However, in recent times the emerging Machine Learning techniques have grabbed the attention of such objectives. Sprung out from Statistics, the ML techniques have seeped into multiple disciplines, including the material science. The cubic X_2YZ half-Heusler compounds are a candidate for spintronics technology [5, 6, 8, 15, 26]. Interestingly, they possess high spin polarisation. The net electron spin magnetic moment in the molecule is an instrumental parameter for spintronics. We are inquisitive to see how well will an ML model closes down to the values calculated from DFT. Especially, after several reports of successful implementation of ML models to improve the thermal properties of materials [17, 19, 20, 23, 24].

The magnetism in a material originates from electron spin and the electron exchange interactions [4, 7, 22]. Indeed due to the double exchange, the compound Cu_2MnAl becomes ferromagnetic, although non of its constituent elements is ferromagnetic by itself [12]. The presence of two different magnetic sublattices in the crystal structure, the XYZ Heusler compounds displays multiple magnetic phenomena, and in fact, today ferromagnetism, ferrimagnetism, and half-metallic ferromagnetism are well studied. Similarly, the half-Heusler, materials exhibit one magnetic sublattice since only the atoms on the octahedral sites can carry a magnetic moment [11]. Understanding these electronic properties has led to breakthroughs.

Another important probe in new material designs and improvements is Elastic modulus. Several physical properties, such as hardness and melting point, are related to the elastic constants [9, 10]. For the Heusler compounds, elasticity has been studied to determine its stability [25]. In this study, it will be the next parameter to predict via the ML model.

As of today, Machine Learning algorithms like Decision trees and Deep neural networks have been applied to classify the Topological insulators [1,3] and topological phases [16]. Moreover, the high accuracy in lattice parameters prediction is demonstrated in multiple studies [2, 13, 27]. Machine learning techniques may soon be poised to compete, or at least corroborate, the results from traditional Computational frameworks. After all, it's robust and requires few and simple training features like atomic configurations and molecular parameters to churn out desired parameters. Incidentally, It's not the everyday choice. However, without any hassle, the input features for any ML model can be easily be engineered for better output. In this paper, we tried to achieve a similar feat on Machine learning-based studies of materials. Traditionally, these calculations are performed via costly DFT.

2 Computational method

Gradient Boosted Trees (GBT) and Artificial Neural Networks (ANN), were put to the work. Two ML models choice provides redundancy in the outcomes. Moreover, GBT was chosen to get rid of the risk for overfitting and ANN for it's high scalability and extensible architecture. Since we were investigating the regression models, the best choice for metric was the R-square. We made the ML model predict the Lattice parameter for a quick showcase of its accuracy. Next, the main task to predict the magnetic moment and the poisson's ratio was performed in the hope for high accuracy. The figure 1. gives a schematic for the model implementation. For the ANN, feature scaling was paramount. Grid-Search was deployed to obtain the best set of hyper-parameters for both models. The dataset was split by 80:20 ratio and a five-fold cross validation was used for a proper metric score. In essence, all the standard procedures was undertaken to build the best ML model. The necessary training datas were obtained from the Python library Pymatgen [18]. However, the list of specimen was taken from the recently published scientific report [17].

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