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Materials Informatics for the Development and Discovery of Future Magnetic Materials

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Abstract—This report summarizes the recent development of magnetic materials search using artificial intelligence (AI) and machine learning (ML). The report briefly introduces ML and AI approaches to materials discovery, and the authors offer a flowchart to aid the selection of relevant approaches for their material search. The report also covers the authors' recent research activities in magnetism and quantum materials, including topological materials, Heusler alloys, interfaces and permanent magnets. This overview is based on a recent symposium at IEEE Intermag 2023.

Index Terms—Half-metallic materials; Hard magnetic materials; Magnetic alloys; Magnetic and spintronic materials.

I. INTRODUCTION

Our society has relied on the discovery and development of functional materials to create new functionality with improved efficiency. For example, a permanent magnet has been improving its energy product, known as BH_{\max} , by moving from binary iron-oxide to more sophisticated Nd-Fe-B magnet [Coe 2020]. In spintronics, a ferromagnetic material with higher spin polarization has been developed [Elphick 2020]. Such research in materials science emerged in the 1990s thanks to the development of vacuum and growth technologies. The collection of these studies created a considerably-sized and reliable database, such as MatNavi [NIMS web] and Springer-Materials [Springer web], which can be accessed and processed via the recent advancement in computational capability. This allows artificial intelligence (AI) and/or machine learning (ML) approaches for the material search, so-called materials informatics (MI) [Hu 2022]. MI was initiated by the Materials Genome Initiative in 2011, which successfully predicted a new electrode for a battery and fabricated it experimentally in the following year. Since then, many initiatives have been introduced by governments and companies to discover and develop new functional materials with high throughputs.

Table 1 summarizes ML methods for materials research. As listed,

some methods do not predict the stability of an alloy, requiring additional calculations of energy to confirm the stability or refer to the corresponding phase diagrams. To guide to select a relevant method, Figure 1 shows a simplified flowchart, illustrating the decision-making process involved in determining the appropriate ML model for investigating the magnetic properties of materials. It is worthwhile mentioning that the choice is never unique, and one task can be accomplished by as many models as possible. The first step entails verifying the availability of an adequate amount of training data with reasonable quality, with the presence of physical descriptors, chosen manually/automatically, that allow the model to learn the underlying physical properties from the given features.

Based on the specific objectives of a study, different types of ML algorithms can be selected, including clustering, classification, regression, and dimensionality reduction techniques. It is important to note that the algorithms depicted in the flowchart represent a small subset of the available options, and researchers have the flexibility to explore additional algorithms based on their specific requirements. Due to the availability of the data labels, either supervised learning (with data labels) or unsupervised learning can be chosen as parallel guidance of the flowchart. For regression problems, supervised learning can be used, while for dimensionality reduction, it belongs to unsupervised learning. Moreover, depending on whether the model complexity grows with the data, we can also guide the choice through parametric models or non-parametric models. Parametric models like NNs or linear regression have more "fixed" model structures and have made assumptions about the data distribution, while

Corresponding author: Atsufumi Hirohata (atsufumi.hirohata@york.ac.uk). R.O., M.L. and A.H. wrote the second chapter, and C.F. wrote the third chapter. The second chapter was written by all the authors individually.
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non-parametric models like random forest, although can still contain parameters, will grow the model complexity when the data size grows. Among these options, NNs stand out as a highly versatile Table 1. List of major AI/ML approaches for material search.

approach for capturing complex features. The architecture of the NN can be tailored to the data representation at hand, enabling effective modeling of intricate relationships between variables.

AI/ML approaches	Advantages	Disadvantages ¹⁾
Neural networks (NNs)	Protected by the universal approximation Theorem, NNs can learn intricate patterns from data including non-linear relationships for arbitrary functions in principle. They enable end-to-end learning, adapted to well-generalized model to capture feature hierarchies.	NNs require a lot of computational resources (<i>e.g.</i> , central processing unit (CPU) with a clock speed of at least 2 GHz and multiple cores, graphics processing unit (GPU) with a base clock frequency of at least 1 GHz or higher [Li 2023]) “Black box” nature can lose the interpretability of the model.
Support vector machine (SVM)	SVM is effective in high-dimensional spaces, even when the number of dimensions is greater than the number of samples.	SVM underperforms where the number of features for each data point exceeds the number of training data samples.
Linear regression	Linear regression is simple and provides a clear, interpretable model structure. With the data size n and number of features d , the training time and training space complexity of linear regression are $O(nd)$, whereas the testing time and space complexity are $O(d)$ [Singh 2022].	It can be sensitive to outliers and may perform poorly with non-linear data or when there are interactions between features.
Logistic regression	Logic regression provides a probabilistic interpretation and it can be regularized to avoid overfitting.	It cannot solve non-linear problems because it is a linear classifier.
K-means clustering	K-means clustering is simple to understand and implement. It is also efficient in terms of computational cost.	It requires to specify the number of clusters, which is not always feasible. It is sensitive to initial conditions and outliers. It also assumes spherical clusters of equal sizes.
K-nearest neighbors	K-nearest neighbors is a non-parametric method and can capture complex patterns in the data.	It is sensitive to the local structure of the data, irrelevant features, and the scale of the data. It does not know which attributes are more important.
Decision trees	Decision trees are simple to understand and interpret. They can handle both numerical and categorical data and can model non-linear relationships.	They can create over-complex trees that do not generalize well from the training data. They can be unstable because small variations may generate a completely different tree.
Random forests	Random forests reduce overfitting problems in decision trees. They can handle large datasets with higher dimensionality. Gradient-boosted trees (GBT), such as XGBoost, can improve the optimization process via a weak prediction model.	They may be seen like a black-box approach for statistical modelers as you have very little control over what the model does. They can be slow to evaluate.
Principal component analysis (PCA)	PCA can simplify a dataset by reducing a large set of variables to a smaller one that still contains most of the information.	The original variables are replaced by a set of principal components, which are not as interpretable as the original data.

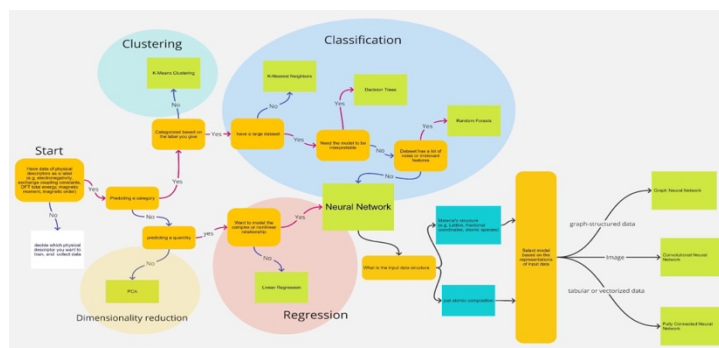


Fig. 1. Flowchart to select an appropriate method for ML.

II. CASE STUDIES

A. Magnetic Ordering

We introduce a research work that focuses on developing a model to predict the category of magnetism based on their crystal structures. The motivation is to enhance our understanding of magnetic materials and enable faster and more efficient discovery of new magnetic

materials for various applications [Merker 2022].

To build the model, we used material structures as input data, which include information such as lattice parameters, atomic coordinates, and atomic species. The material structures were converted into graph structures in a graph neural network (GNN). Intuitively, a GNN can be considered as a more flexible version of the more common convolutional NN, where each pixel and its neighbors ex-

perience convolution operation with a mask function. In a GNN, graph nodes and the neighbor nodes perform similar operations. In this example, the desired output of the model is the class of magnetism exhibited by the material. For magnetic propagation vector classification, we collected 1,562 material structures with known magnetic properties from experiments to train and validate the model. NN was chosen as the model architecture due to its ability to incorporate complex interactions present in the materials. For magnetic order classification, a larger density-functional-theory (DFT)-based database from Materials Project [Jain 2013] is used. Compared to other methods such as decision trees, NNs can capture intricate relationships between input features and output labels, even in cases where it is challenging to separate the contributions to magnetism from different factors. In particular, we utilized a specialized NN called GNN for their model architecture. GNNs are well-suited for modeling material structures as crystal graphs, and in this particular case, with added symmetry to the GNN, it allows for the inclusion of Euclidean symmetry considerations.

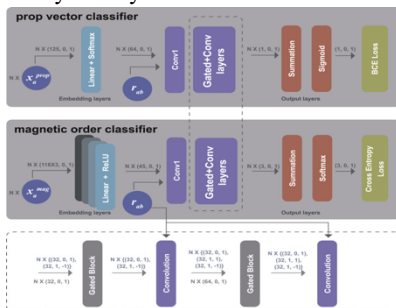


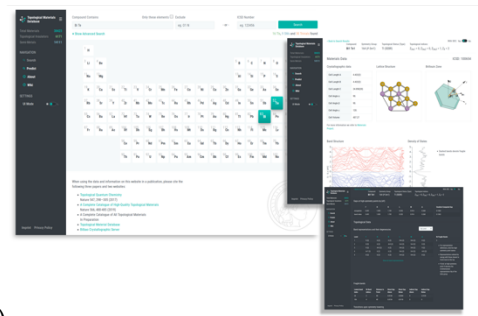
Fig. 2. Illustration of the neural network architectures for propagation vector (top block) and magnetic order classification [Merker 2022].

The results demonstrate the effectiveness of the developed model in predicting the category of magnetism with an average accuracy of 77.8%, and with 73.6% for propagation vector prediction. By training the model on a large dataset of material structures, it achieved high accuracy in correctly classifying the magnetic properties of new materials. This suggests that the model is capable of capturing the complex relationships between material structures and their magnetic behaviors, though there is still room for further improvement. The findings contribute to the field of materials science by providing a valuable tool for predicting magnetism in various materials, thereby facilitating the discovery and design of new magnetic materials.

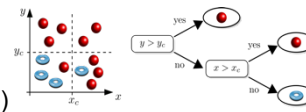
B. Topological Properties

Topological insulators (TIs) or topological semimetals (TSMs) are condensed matter systems exhibiting robust edge or surface modes and quantized bulk response functions due to the topological properties of their electronic wavefunctions. The advent of symmetry-based indicators probing topology or topological quantum chemistry allowed the creation of large catalogs of topological materials [Vergniory 2019], with high throughput DFT calculations [Vergniory 2022]. The graphical user interface (GUI) is shown in Fig. 3(a). Predicting topology through ML faces several challenges: a relatively small dataset (in this study 38,298 stoichiometric unique compounds), the outcome being a label rather than an “energetic” quantity and the usage of unstructured features. Our results [Claussen 2020] use a simplified approach based on GBTs, an improved version of the binary tree classifiers depicted in Fig. 3(b),

though some other approaches such as those based on x-ray absorption data to predict topological class also exist [Andrejevic 2022].



(a)



(b)

Fig. 3. (a) Illustration of the neural network architectures for propagation vector and (b) magnetic order classification [Merker 2022].

Our ML model can predict the DFT-computed topology of a given material with an overall accuracy of almost 90% (based on the F1 score, a measure of the accuracy of a test). A breakdown per type of topology shows that our classifier outperforms for trivial materials (F1: 94%) and TSMs (F1: 92%) and underperforms for TIs (F1: 70%). This latest score is a consequence of the imbalance of training sample size between these different categories. Still, our analysis sheds light on the most relevant features that are required to obtain a predictive model. For example, the positions of the atoms do not improve the F1 score. Additionally, GBTs (or simplified versions of them) offer a unique perspective on how the classification is performed. For example, it finds back rules that predict when a system should host a topological surface mode (TSM) based on the number of valence electrons and space group.

C. Interfacial Properties

Magnetic tunnel junctions (MTJs) have been utilized as the read-out head of magnetic storage devices and as the memory cell of nonvolatile magnetoresistive random access memories (MRAMs). An MTJ is composed of two ferromagnetic electrodes separated by an insulating barrier and the resistance of MTJ depends on the relative magnetization direction of the electrodes. In this study, by using *ab-initio* calculations with the aid of ML, we explored MgO-based MTJs, which exhibit high tunneling magnetoresistance (TMR) ratio at room temperature [Shirai 2023]. We focused on quaternary Heusler alloys, $XX'YZ$, where X , X' and Y denote transition-metal elements and Z represents main-group elements. We employed light gradient-boosting machine (LightGBM, based on decision trees) [Ke 2017] for a predictor and considered atomic number, atomic radius, valence-electron number, electron affinity, ionization energy, and thermal conductivity of each element in $XX'YZ$ for descriptors.

First, we explored $XX'YZ$ having higher Curie temperature (T_C) to suppress thermal fluctuation of magnetic moments at room temperature. We performed *ab-initio* calculations for about 4,500 sorts of cubic and tetragonal $XX'YZ$ composed of randomly selected elements. We successfully constructed an ML model to predict T_C of $XX'YZ$. Figure 4 shows the result of regression analysis for T_C of $XX'YZ$ ($>1,000K$). We obtained a relatively high correlation between

predicted and *ab-initio* values, the accuracy of prediction: ~80%. We carried out a virtual screening of $XX'YZ$ having higher T_C among whole candidates of about 100,000 sorts. As a result, we found that about 350 sorts of $XX'YZ$ possess $T_C > 800$ K.

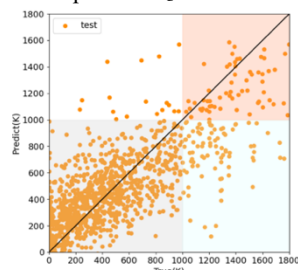


Fig. 4. Correlation between T_C predicted by ML (vertical axis) and that obtained by *ab-initio* calculations (horizontal axis) for $XX'YZ$.

Next, we explored $XX'YZ/MgO(001)$ junctions having higher exchange stiffness at the interface to prevent thermal fluctuation of magnetic moments in the interfacial region. We developed a ML model to predict the interfacial magnetic stiffness by using the *ab-initio* data for about 600 sorts. The regression analysis revealed that the correlation coefficient between the predicted and *ab-initio* values is 0.70 for test data. As a result of virtual screening, we found the junctions composed of inverse Heusler alloys Fe_2CoZ ($Z=Al, Ga$ and In) have higher stiffness at the FeZ -terminated interfaces with MgO .

D. New Magnetic Materials

Highly magnetic materials are critical in the manufacturing of information storage systems, motors, sensors, actuators, and other electronic devices. Traditionally, the binary alloy Fe_3Co with the highest magnetization among stable alloys (referred to as the Slater-Pauling limit [Kakehashi 2012] depicted in Fig. 5(a)) has been used. However, efforts are ongoing to discover alloys with magnetization that surpass this limit. These investigations focus on multi-element alloys, but their combinatorial explosion requires numerous simulations and experiments, making comprehensive studies challenging.

Addressing this issue, we used an autonomous materials search system, combining ML and *ab-initio* simulations, to examine multi-element materials [Sawada 2018]. Figure 5(b) shows the autonomous system, which mimics the traditional process of manual materials search including fabrication of materials (step A), evaluation of properties (step B), and deciding on the next target materials (step C). Steps A and B are virtually simulated by *ab-initio* calculation, predicting material properties from the composition and crystal structure information. Bayesian optimization assists in deciding the next target composition/structure (step C). This procedure balances the exploration of new materials and exploitation of known information, allowing for the selection of target materials with better properties. With each cycle, the increase in learning data progressively refines the ML model, leading to suggest superior materials.

The autonomous materials search system was operated continuously over a period of 9 weeks. The system's progressive development is visually captured in Fig. 5(c), wherein data representing the magnetic moment of materials that the autonomous system tried is plotted for each cycle. As the system accumulated learning data, it became increasingly proficient in proposing alloy compositions exhibiting greater magnetic moments. Importantly, the system demonstrated its strategic approach by intermittently testing alloy

compositions with diminished magnetic moments. This strategy highlights the system's capacity to balance the exploration of new possibilities with the exploitation of known data throughout the multifaceted virtual search. After six weeks, the system proposed an alloy with the highest recorded magnetic moment, $Fe_{82}Co_{13}Ir_4Pt$. This alloy, dominated by Fe and Co, surprisingly also contains small amounts of Ir and Pt, elements typically associated with low magnetic moments. The performance of these alloys was confirmed by both experiments and theories [Iwasaki 2021]. Our autonomous materials search system for materials discovery is quite versatile and can be used in the development of various materials.

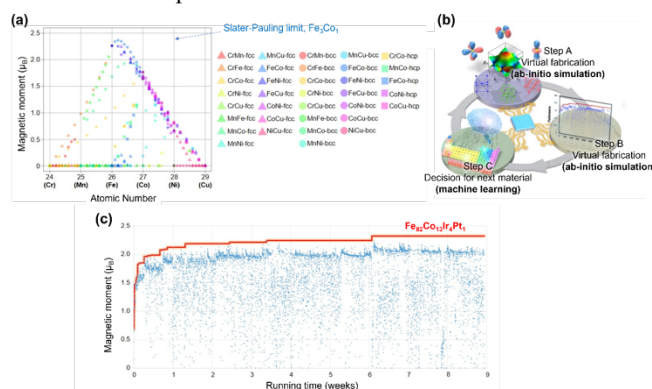


Fig. 5. Discovery of high-magnetization alloy by autonomous materials search system combining *ab-initio* calculation and ML. (a) The Slater-Pauling curve. (b) Autonomous materials search system in which the conventional process of materials search is simulated using computation technologies including *ab-initio* simulation and ML. (c) Growth of the autonomous materials search system for an alloy with a large magnetic moment [Iwasaki 2021].

E. New Permanent Magnets

A method similar to case study D was used in the first part of this study. It involved using regression and principal components for dimensionality reduction to create a model. This model (ML1), partial least squares regression (PLSRegression [Höskuldson 1988]), could predict the intrinsic material properties of permanent magnet materials, spontaneous magnetization $\mu_0 M_s$ and uniaxial anisotropy constant K_u , based on the chemical formula of the 2-14-1 system [Marinescu 2002]. The training data came from an experimental database and was further enhanced with a large database of DFT calculations for different chemical combinations of the elements, Nd, Pr, La, Ce, Ni, Fe, Co and B, within the same system. When a magnet engineer/developer needs to find the most suitable material combination for their application, they can use this trained model inversely. Such that they solve an optimization problem with the trained model to identify the best material candidates while carefully considering the model's confidence intervals for each prediction.

Furthermore, the study combined this model (ML1) with another model (ML2) operating at a larger length scale, a model that predicts the coercive of the permanent magnet. This single grain model, a shallow neural network, predicts the coercive field based on the geometrical parameters of a single core-shell-grain-boundary grain and the chemical composition of the three phases involved. By doing so, multi-objective optimizations become feasible, allowing scenarios where coercivity needs to be maximized while simultaneously minimizing costs. For instance, this could be applicable when deal-

ing with unavoidable defects, such as a fixed thickness of a defect shell around the grains, like 5 nm (large defect) or 2 nm (thin defect).

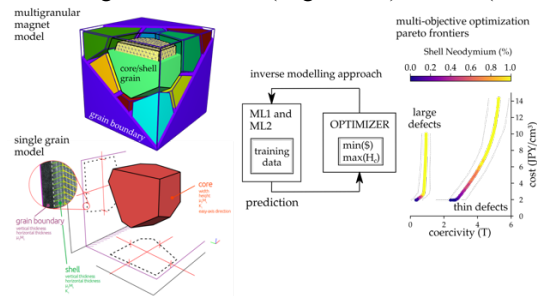


Fig. 6. Sketch of multi-objective optimization scheme, in which geometrical parameters and intrinsic material properties of a single grain model are optimized. The right shows two optimization results, two Pareto frontiers, one with a thin defect and one with a thick soft magnetic defect shell surrounding a single grain [Kovas 2022].

Model (ML1) has been trained with 200 experimental entries of chemical composition and anisotropy field measured at different temperatures (300–473K). It has been combined with data from first-principles simulations including exchange integral values, such as approximations of the magnetic moment at 0K, T_C and lattice constants along the same chemical concentration of 2-14-1 systems. Model (ML1) after training achieves a coefficient of determination (R^2 score) of 0.961 in which the mean absolute error for magneto-crystalline anisotropy constant is 0.31 MJ/m³ and 0.04 T for the saturation magnetization. Model (ML2) achieves $R^2=0.975$ and a mean absolute error of 0.15 T for predicting coercivity [Kovas 2022].

III. CONCLUDING REMARKS

We have reviewed major AI/ML approaches available in the study on magnetic materials and devices. The flowchart offers a simplified way to select an appropriate approach for a certain subject. These AI and ML approaches have shown great promise in predicting new materials with specific properties, but they hold several limitations that researchers must keep in mind. (i) *Data availability*: Machine learning models require large amounts of high-quality data to make accurate predictions. In materials science, there are limited data available for certain types of materials or properties. Symmetry-aware NNs is one promising approach to reduce the data intensity. (ii) *Quality of data*: Even when data is available, it is not of high quality or may contain errors or biases that can impact the accuracy of machine learning predictions. To improve the quality, data pre-screening, anomaly detection, noise reduction can be performed as standard practice. (iii) *Interpretability*: Machine learning models are often considered “black boxes”, which can make it challenging for researchers to understand how the model arrived at a particular prediction. For this, interpretable ML is making rapid progress. (iv) *Computational requirements*: The computational resources required to train and run machine learning models can be substantial, which may limit their accessibility to those with limited resources.

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