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## Machine Learning Applications for Materials Science: Predicting Properties of Two-Dimensional Magnetic Materials

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## Machine Learning Applications for Materials Science: Predicting Properties of Two-Dimensional Magnetic Materials

### Abstract

We trained successful neural networks to predict the formation energy and magnetic moment of 2-dimensional ferromagnetic materials of similar structure to Cr<sub>2</sub>Ge<sub>2</sub>Te<sub>6</sub>. We collect elemental data on materials with known and unknown properties from easily accessible sources to screen for viable materials for use in future research. Random forest regressors were used to identify the most important predictors of our target qualities, which perform better on predictions of formation energy than magnetic moment. We predict the properties of 1225 materials that are candidates for further research in two-dimensional magnetism and identify several potential sources of error in our models that can be targeted for further improvement.

## I. Introduction

Two-dimensional ferromagnetic materials are a relatively recent and surprising discovery, as long-range ferromagnetism was previously thought to be heavily suppressed in two dimensions according to the Mermin-Wagner theory. This theory posits that long-range magnetic order in two dimensions is easily disrupted by thermal fluctuations and requires magnetic anisotropy, where the magnetic field is directionally dependent. Magnetic anisotropy implies spontaneous symmetry breaking, as applying an external field to an anisotropic material can magnetize it in either direction along its preferred axis. Gong et al. (2017) present  $\text{Cr}_2\text{Ge}_2\text{Te}_6$  as a two-dimensional material and demonstrate control over its shift between paramagnetism and ferromagnetism in laboratory-achievable temperature and magnetic field conditions.

The discovery of such materials has important applications for the understanding of the origins of long-range magnetism as well as for devices. Data storage through magnetoresistive random access memory (MRAM) uses magnetic resistance generated through a junction of magnetic materials instead of traditional electrical junctions, such as in transistors, to store data. Two-dimensional materials are a promising pathway to shrink such devices and improve storage density. Other applications of these materials exist in optics and magneto-optics, such as the generation and control of lasers and photodetectors.

Machine learning offers a faster and computationally less expensive means to identify potential materials of interest. Materials for study must be thermodynamically stable and magnetic to be useful for research or devices. Density functional theory (DFT) is commonly used to compute these properties prior to investing in experimentation, yet is costly in both time and computational power which limits the breadth of materials that can be considered as candidates. Machine learning models trained on materials with known qualities and descriptors can be used instead to estimate the properties of untested materials. This allows for much more rapid screening of long lists of candidate materials, and materials predicted to have the desirable qualities can be selected for further investigation. With  $\text{Cr}_2\text{Ge}_2\text{Te}_6$  as a template, Rhone et al. (2020) present 223 potential materials and demonstrate that machine learning models can successfully predict key material properties from various elemental descriptors. This study builds upon their work and predicts on 1225 similarly structured materials to identify materials in two-dimensions likely to be stable and ferromagnetic.

## II. Methods

We trained neural networks and random forest regressors on a dataset of 223 2-dimensional materials provided by Rhone et al. (2020). These materials follow an  $\text{A}_2\text{B}_2\text{X}_6$  pattern modeled after  $\text{Cr}_2\text{Ge}_2\text{Te}_6$ , where the A-site is populated by transition metals, the B-site with p-block atoms, and the X-site with tellurium atoms (Figure 1). Each material has at least one chromium atom in the A-

sites. We first trained neural networks on the 67 atomic properties, henceforth called ‘descriptors’ of the materials, provided by Rhone et al. (2020) to establish expectations for model performance before assembling similar datasets.

We collected atom-wise descriptors on each material from the package mendeleev version 0.4.1 including atomic radius, electronegativity, number of electrons and electron configuration, and computed statistics such as the mean and standard deviation of the values and their differences for a total of 58 descriptors. Due to data availability, material-scale descriptors such as total energy and spin were not included, unlike the dataset provided by Rhone et al. (2020). Our models predicted formation energy of the material as a proxy for thermodynamic stability and magnetic moment for bulk magnetism. These predictions were then compared to the DFT-calculated values provided by Rhone et al. (2020). We used 60 percent of the data for training, 20 percent for validation, and 20 for testing for each model before predicting on the set of 1225 new materials.

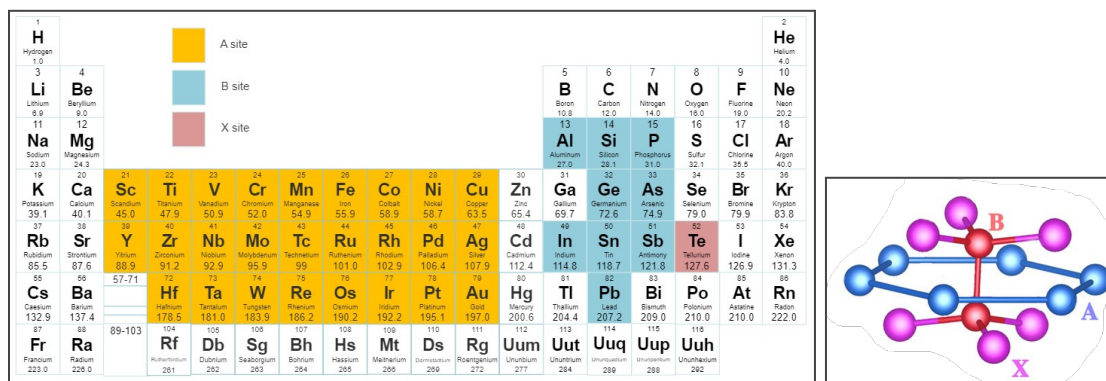


Figure 1a (left). Periodic table of the composite elements of the materials studied. Figure 1b (right). Unit cell of an  $A_2B_2X_6$  material (source: Rhone et al. 2020)

Following the same  $A_2B_2X_6$  structure with the same distribution of elements, we assembled descriptors for 1225 theoretical materials and predicted their formation energies and magnetic moments. In general, neural networks are more flexible models able to find complex relationships between descriptors and target variables. However, the complicated relationships between variables in neural networks make it difficult to identify which descriptor variables are most useful in predicting targets and the architecture of the model is challenging to interpret. Neural networks are also prone to overfitting given the large number of trainable parameters and perform best on large datasets. These models performed best when using an exponential linear unit, or ‘elu,’ activation function instead of the more common ‘relu,’ or rectified linear unit, activation. The activation function of a neural network determines the response of each neuron in the model to its respective inputs. Models activated with ‘elu’ functions allow negative values to be passed between

layers which adds model flexibility and reduced underfitting, particularly in our magnetic moment models.

We trained random forest regressors to address some of the shortcomings of neural networks, as descriptor importance is easily obtainable from such models and the ensemble nature of random forests helps to limit overfitting. Random forests are preferable to regularized linear models in this study due to the non-linear relationships between our descriptors and targets, particularly for magnetic moment predictions. The relatively small size of our training dataset of 223 samples also risks high variance, wherein minor changes to the random initialization of training-testing splits or starting parameters can greatly affect the performance of the resulting model. Random forests tend to outperform linear models in these circumstances by averaging the result of many smaller models and thus reducing the threat of variance.

### III. Results and Discussion

#### Formation Energy

Models trained and tested on the original dataset provided by Rhone et al. (2020) produced testing  $R^2$  scores of 0.93 and 0.84 for formation energy and magnetic moment predictions, respectively (Figure 2).

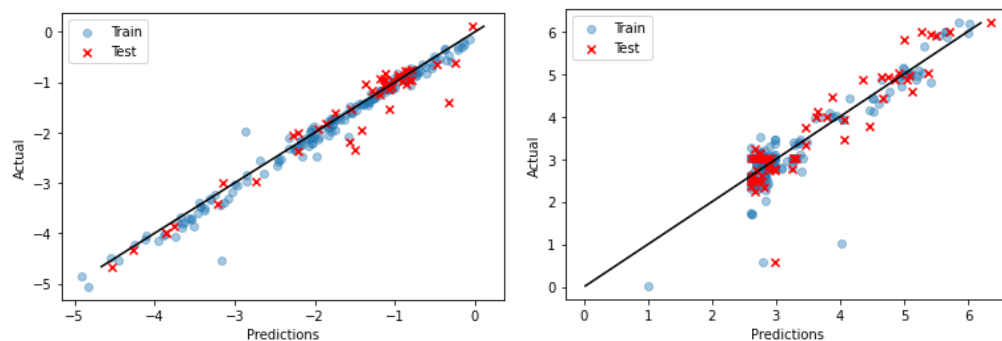


Figure 2. Neural networks predicting formation energy (left) with a testing  $R^2$  score of 0.93 and magnetic moment (right) with a testing  $R^2$  score of 0.84, trained on the original dataset from Rhone et al. (2020). The DFT obtained value is shown on the vertical axes and the model prediction is shown on the horizontal axes. Samples used for training are indicated with blue circles while testing samples are shown as red crosses, and the black line indicates where the predicted value is equal to its DFT calculated counterpart.

Our formation energy neural network trained on the newly prepared dataset performed similarly, achieving a  $R^2$  score of 0.94 (Figure 3). This model was less accurate on materials with formation energies near the top and bottom of the range. This may indicate that the model is underfitting the data and requires additional tuning, or that some of the descriptors omitted in the new data but included in the dataset from Rhone et al. (2020) are key to higher and lower values of formation energy.

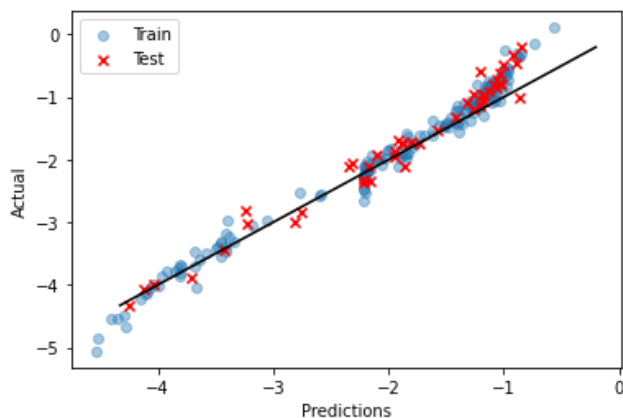


Figure 3. DFT calculated values vs. neural network predictions of formation energy on the 223 materials provided by Rhone et al (2020).

The random forest model was also successful with a  $R^2$  of 0.95 and better predictions for materials with higher and lower formation energies (Figure 4a). For formation energy, the small size of the training dataset may be limiting performance and the additional flexibility provided by neural networks does not appear to be necessary to capture relationships between the descriptors and the target. We find that the strongest coefficients to predicting formation energy are the number of electrons in the d-orbitals, the standard deviation of atomic electronegativity, and the average dipole polarizability (Table 1). Since only atoms in the A-site of the materials have incomplete d-orbitals, our results suggest that the composition of the A-site has a large bearing on the formation energy of the material. Our results do not match those of Rhone et al. (2020) where they find atomic radius and volume to have significant impact on formation energy. We find instead that the dipole polarizability of the constituent atoms and the differences between them are key predictors, which may be due to electric attraction between atoms. Given the similarity between the random forest predictions and the neural network (Figure 4b) and the accuracy of them both, it is reasonable to extrapolate our findings on descriptor strength from the random forest model to the neural network.

Our neural network was used to predict on the set of 1225 new materials. The five materials with the most and least negative formation energies are shown in Figure 5. As would be implied by the descriptor strengths found by the random forest, A-site atoms with few d-orbital electrons such as yttrium and scandium are popular in materials with the most negative formation energies,

while atoms like copper with nearly full d-shells appear amongst the least negative formation energies. More empty slots in the valence shell appears to reduce formation energy and thus produce more stable materials, likely due to the propensity of these atoms to form covalent bonds.

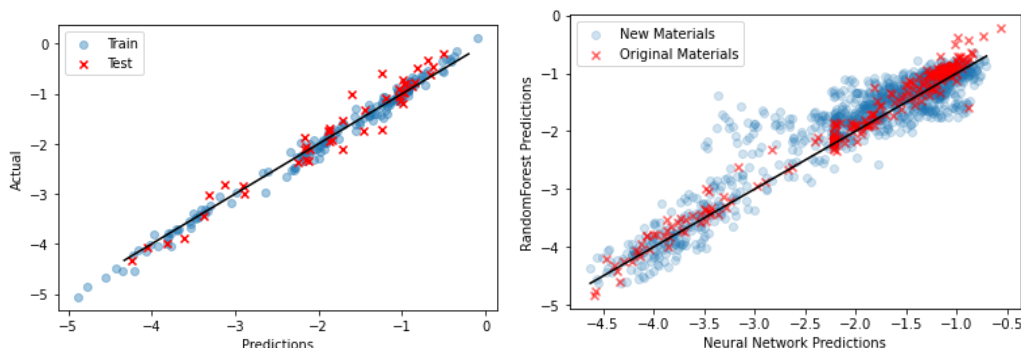


Figure 4a (left). DFT calculated values for formation energy vs. random forest model predictions for the 223 sample materials included in Rhone et al. (2020). Figure 4b (right). Comparison of neural network and random forest predictions on the training data, in blue, and new materials, in red. The poor performance of the model near the center of the formation energy range can be attributed to the dearth of training samples in the region.

Rank	Descriptor	Rank	Descriptor
1	d-orbital electrons (sum)	5	d-orbital electrons (max. difference)
2	electronegativity (standard deviation)	6	electronegativity (mean)
3	dipole polarizability (mean)	7	dipole polarizability (max. difference)
4	electronegativity (max. difference)	8	dipole polarizability (stan. dev. of differences)

Table 1. Strongest random forest descriptors for formation energy, in order of descending coefficient absolute value. The first-ranked descriptor was roughly twice as strong as that of the second-ranked descriptor.

### Magnetic Moment

The neural network trained and tested on the newly assembled descriptors modestly outperformed the model trained on the dataset provided by Rhone et al. (2020), with a  $R^2$  score of 0.87 (Figure 5a). However, training and testing the same model (i.e. with the same architecture and hyperparameters) on a different train-test split of the data yielded a  $R^2$  of only 0.76. This suggests

that the model still suffers from high variance, though even the re-trained model is likely sufficient for identifying candidate materials for future study. Figure 5a shows several stark outliers where predictions differ greatly from the DFT values, and the worst predictions are shown in Figure 5b. We examined the predictions for the highest and lowest magnetic moments in Figure 6 and found that molybdenum is common amongst the materials with the largest DFT calculated magnetic moments, while vanadium is present in three out of the eight materials with the smallest magnetic moments and the presence of niobium similarly implies a low magnetic moment.

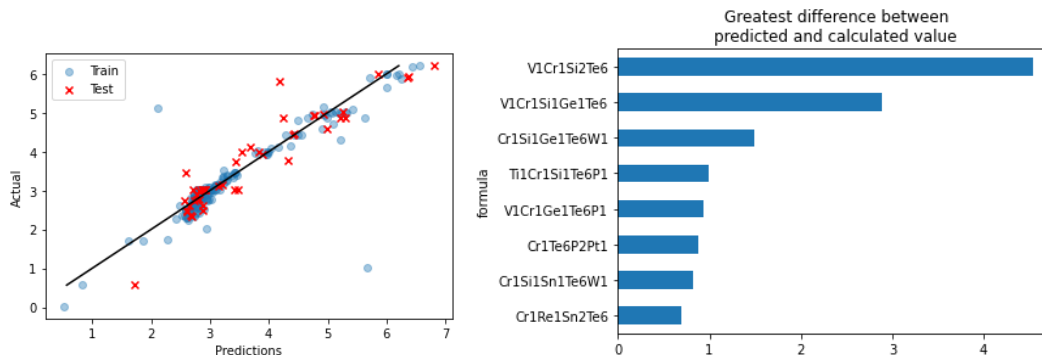
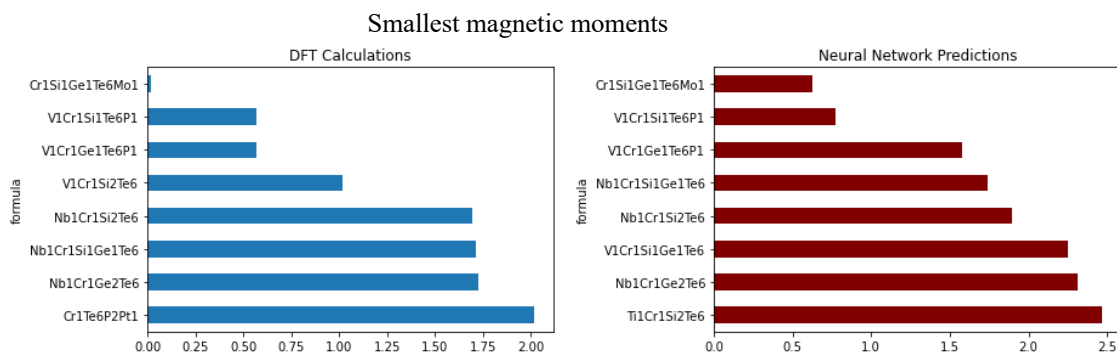


Figure 5a (left). DFT calculated values for magnetic moment vs. neural network predictions for the 223 sample materials included in Rhone et al. (2020). Figure 5b (right). The absolute value of the difference between the DFT calculated value and the model predict of the eight worst material predictions.



Largest magnetic moments



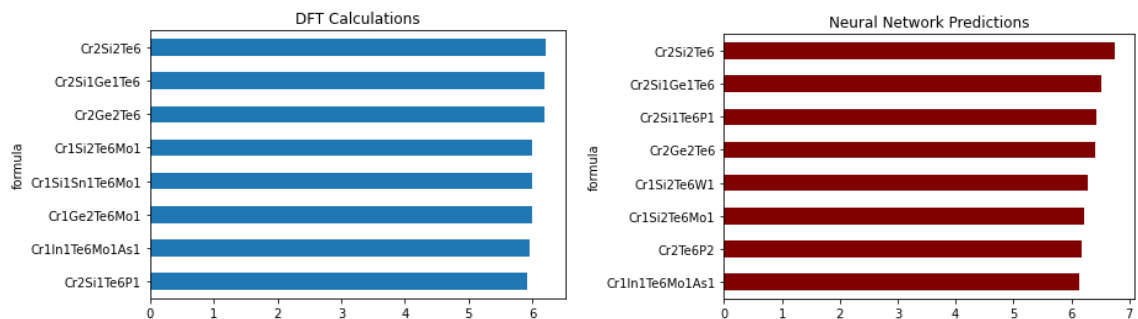


Figure 6. The eight smallest (top) and largest (bottom) magnetic moments from DFT calculations (left) and neural network predictions (right). The model correctly predicts many of the strongest and weakest magnetic moments, suggesting that it is capable of predicting values on the range edges.

A random forest regressor was also trained on the new data, though its performance was underwhelming at a  $R^2$  of 0.70 (Figure 7a). Compared to the neural network (Figure 7b), the random forest failed to model the whole range of magnetic moment values and underfit the data. Its poor performance likely limits the usefulness of considering descriptor importances, since it does not adequately represent the relationships between the descriptors and magnetic moment. Despite this, we found in agreement with Rhone et al. (2020) that the number of valence electrons and the number of unpaired electrons are important predictors of magnetic moment. The magnetic dipole moments of unpaired electrons contribute to the overall ferromagnetic quality of the material, as expected. Our strongest descriptor was found to be the maximum difference between atoms in the number of d-orbital electrons, with a negative coefficient. As observed in the prevalence of Cr<sub>2</sub> and CrMo in the largest DFT-calculated magnetic moments, this suggests that having both A-site atoms with the maximum amount of unpaired d-orbital electrons is a strong contributor to overall magnetic moment. Omitting certain descriptors may have adverse effects on our model performance. The second most important descriptor found by Rhone et al. (2020), chemical space bag of bonds, was not able to be included in this study and this discrepancy may account for some of the differences observed in our model.

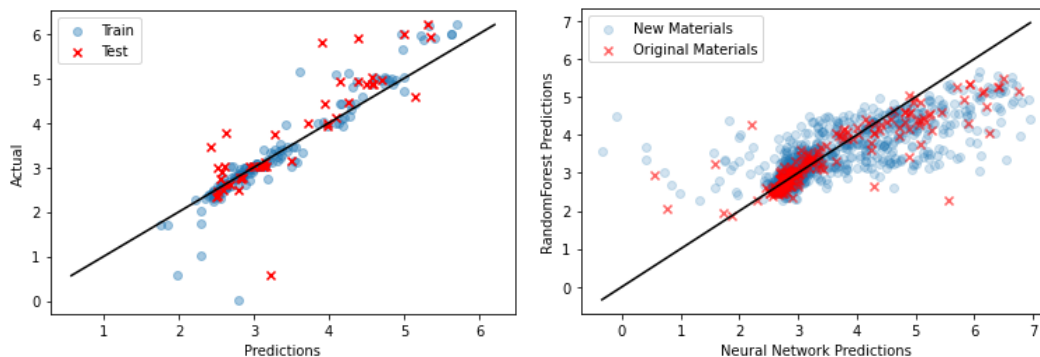


Figure 7a (left). The DFT calculated values of magnetic moment vs. random forest regressor predictions.

Training samples are shown in blue and testing samples in red, with all samples coming from the set of Rhone et al. (2020). Figure 7b (right). Comparison of the random forest predictions to the neural network predictions on the expanded dataset of 1225 materials. The materials studied by Rhone et al. (2020) are displayed in red and the new materials are in blue.

Rank	Descriptor	Rank	Descriptor
1	d-orbital electrons (max. difference)	5	number of valence electrons (mean)
2	number of valence electrons (standard deviation)	6	electron affinity (mean)
3	number of unpaired electrons (sum)	7	electronegativity (sum of differences)
4	number of unpaired electrons (mean)	8	number of electrons (mean)

Table 2. Strongest descriptors of magnetic moment according to a random forest regressor.

Figure 8 presents the six materials from our expanded sample list with the greatest and least magnetic moments. These predictions match patterns observed in our predictions on the smaller training dataset, where materials containing two chromium atoms are predicted to have large magnetic moments and vice versa for materials containing molybdenum. However, Figure 6 suggests that molybdenum is common amongst materials with strong magnetic moments, so these predictions should be re-evaluated prior to screening out molybdenum-containing materials for further study. These predictions should be compared with other successful models and the neural network requires further optimizations to be confidently used as a screening tool for all materials. The random forest specifies derivations of the number of d-orbital electrons and the number of valence electrons to be the strongest predictors of magnetic moment, of which chromium and molybdenum have the same number. This implies that either the neural network is not adequately identifying the relationship between these descriptors and magnetic moment, or the random forest regressor is incorrectly selecting the most important descriptors.

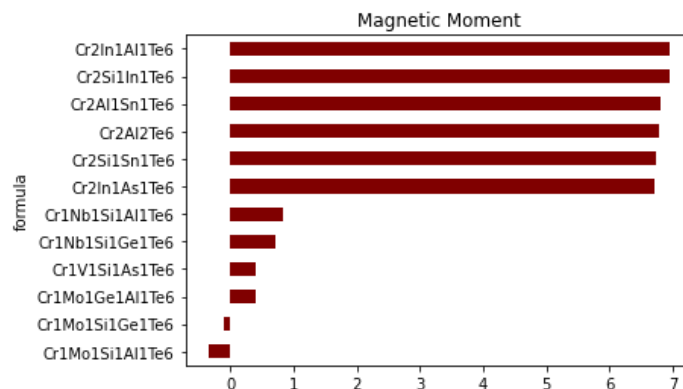


Figure 8. The six materials with the largest predicted magnetic moment and the six materials with the smallest magnetic moment.

#### IV. Conclusions and Future Work

We trained successful neural networks to predict formation energy and magnetic moments on the list of materials studied by Rhone et al. (2020) and extrapolated our models to 1225 new materials to identify candidates for further research. We found the most important atomic-wise descriptors for the prediction of formation energy which can guide future materials discovery. More work should be done on models of magnetic moment that provide insights into feature importance in order to isolate the best predictors of this property. Our models in their current state are already useful for initial candidate material screening with low time and computation cost, so can be used on larger selections of materials to guide further studies.

Particularly for magnetic moment, the lackluster performance of the random forest regressor and the mischaracterization of certain materials by the neural network may be attributable to the relatively simplistic descriptors dataset-- in this case, additional model tuning alone would not be sufficient. The benefits of simple atom-wise data is that it is easily and quickly accessible to collect for thousands of materials at a time, and gives easily interpretable results. Including more complex data presents more practical difficulties yet may yield significantly improved results. For example, crystal graph convolutional neural networks (CGCNNs) use atomic properties and graphical bond representations as descriptors and have been found to be comparably accurate in predicting formation energy as DFT calculations themselves, when compared to experimental values. However, CGCNNs require specialized data formats and model architecture that limits their accessibility. We attempted and failed to access adequate datasets for CGCNNs, which is why they could not be included in this study.

The models presented here may also benefit from descriptors such as spin data and chemical space, which are reported by Rhone et al. (2020) to be important predictors of magnetic moment. Unlike the atom-wise descriptors, some of this data may require additional calculations

and thus slow down the predictive process on new materials. However, the machine learning process of selecting candidate materials is already significantly faster than performing computations. The DFT calculations for the 223 materials provided by Rhone et al. (2020) took six months to complete with a supercomputer; in contrast, collecting the descriptors and making formation energy and magnetic moment on the expanded materials list of 1225 required less than twenty minutes on a standard laptop. The time and computational cost of additional descriptors must be weighed against the possible gains to modeling power. Future models should also strive to distinguish between ferromagnetic and antiferromagnetic materials, an important property in many device and research applications.

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