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ABSTRACT

Technologies that function at room temperature often require magnets with a high Curie temperature, T_C, and can be improved with better materials. Discovering magnetic materials with a substantial T_C is challenging because of the large number of candidates and the cost of fabricating and testing them. Using the two largest known datasets of experimental Curie temperatures, we develop machine-learning models to make rapid T_C predictions solely based on the chemical composition of a material. We train a random-forest model and a k-NN one and predict on an initial dataset of over 2500 materials and then validate the model on a new dataset containing over 3000 entries. The accuracy is compared for multiple compounds' representations ("descriptors") and regression approaches. A random-forest model provides the most accurate predictions and is not improved by dimensionality reduction or by using more complex descriptors based on atomic properties. A random-forest model trained on a combination of both datasets shows that cobalt-rich and iron-rich materials have the highest Curie temperatures for all binary and ternary compounds. An analysis of the model reveals systematic error that causes the model to over-predict low-T_C materials and under-predict high-T_C materials. For exhaustive searches to find new high-T_C materials, analysis of the learning rate suggests either that much more data is needed or that more efficient descriptors are necessary.

Ferromagnetic materials are essential in modern technologies especially in energy production and data storage. The threshold temperature where magnetism disappears is called the Curie temperature, T_C. Searches for high-T_C materials typically look for magnets with a T_C of at least 550–600 K, which is required for reliably running an application at room temperature.[1,2] High-T_C magnets are valuable but rare,[1,3,4] in particular when other electronic structure properties are required.[5] Although some empirical rules for the design of new magnets exist,[6] rapid predictions of Curie temperatures could assist in identifying candidate high-T_C magnets in large-scale screening exercises. Thousands of known ferromagnetic materials exist,[7] and while high-throughput computation can help in identifying hundreds of thousands of potential magnets, experience suggests that only a fraction of them can actually be realized.[3,8–10]

Measuring the Curie temperature of a compound is a relatively standard and accurate procedure, but of course needs the material to be made first. In contrast, in a computational design process, the T_C must be predicted ahead of experiments, only using physical and chemical information. This is a complex task prone to large errors. In fact, one needs to compute the elementary magnetic excitations of a compound, most typically from density functional theory (DFT), map these on a simple model, usually a Heisenberg-type one, and then perform thermodynamic sampling with Monte Carlo methods.[11–26] Then, the choice of DFT functional, the quality and appropriateness of the mapping, and subtleties in the Monte Carlo algorithms, all contribute to a large uncertainty on the predictions. Often this uncertainty is so severe that blind predictions of T_C for unknown compounds are almost impossible to make.

Machine-learning algorithms capture complex relationships in data that may be difficult to recognize or understand.[27] Even though machine-learning models often have low interpretability, they can provide cheap Curie temperature predictions. Rapid predictions can be a first step in screening computer-suggested materials so that experimental efforts can be more selective.

Algorithms, such as ridge regression, kernel ridge regression, neural networks, and random forest, have been trained on experimental

data and used to predict Curie temperatures.[1,8,10,28–33] Most of these studies were limited to specific structural or chemical families and used a relatively small dataset (<1800) for training which limited the ability to generalize the results to other less known families. In this work, a random-forest model is trained on an initial dataset of the chemical compositions of over 2500 ferromagnetic materials.[1] We then used a larger dataset of ~3100[7] for a "blind test," which shows our model to have good generalization. Then, we built a model using the combined dataset. This is, by far, the largest dataset to be used in this kind of study.

In general, the crystal structure affects the Curie temperature and there have been attempts to incorporate structural information into different machine-learning models with varying degrees of success. In some cases, Curie temperature predictions that utilize known structural data are more accurate, in particular, when the structural diversity present in the dataset is limited.[7,8,28,30,35–37] However, the use of structural information in a larger and more diverse set of data may have an adverse effect on the T_C predictions.[1] Furthermore, the lack of available structural information excludes a large portion of experimental data, which weakens the model's predictive power. The use of structural data in training a machine learning model also limits predictions to materials with known structure. In this work, we avoid these problems and exploit our large corpus of magnetic data in DS1 and DS2 by using models and data that do not include structural information.

In Ref. 1, a random-forest model was used to predict the Curie temperature based solely on chemical composition. In this work, we first use the same data (DS1) and attempt to improve the predictions by trying different machine-learning models and alternate descriptors. Using the random-forest model trained on DS1 to make predictions on a new set of experimental data (DS2),[7] we find that the model generalizes quite well but the prediction errors are 90 K (MAE) as compared to 69 K (MAE). Next, we combine DS1 and DS2 to build a new model and scan over hundreds of thousands of potential new magnets. In the process, we find that the errors between the experimental and predicted Curie temperatures reveal a previously unnoticed systematic error.

We cleaned both DS1 and DS2 according to the methods outlined in Ref. 1. Both datasets had many duplicate compounds often with different reported experimental Curie temperatures. The duplicates were eliminated by selecting only the median Curie temperature in order to retain an actual measured value of the T_C. In DS1, we also added entries for each of the non-magnetic elements found in the data and set the Curie temperature to zero. After cleaning the raw data, DS1 contains the Curie temperatures of 2557 unique compounds and DS2 contains 3194. There is an overlap of 1189 compounds between DS1 and DS2. Our feature vector has 85 features, each one describing a distinct element found in the data. Each compound is characterized by placing the percentage that each element occupies in the compound in the appropriate feature. For each machine-learning prediction, a randomly selected third of the compounds in DS1 was used as the test data and the other two thirds were used to train the models.

It is not possible to visualize the data in 85 dimensions. However, a t-distributed stochastic neighbor embedding[34] (t-SNE) projection reduces the data to two dimensions and may reveal data clustering. Figure 1(a) shows the t-SNE plot for DS1, where each point is colored by the majority element in the compound. The red circles show areas where compounds with the same majority element cluster together. Figure 1(b) shows the same t-SNE plot but with the colors corresponding to the Curie temperatures of each compound. Each point in these plots represents a magnetic compound in the dataset. A comparison of the two plots reveals that most of the high-T_C materials have a majority element of either cobalt or iron. It also shows that there are occasional high-T_C spikes in clusters, where the T_C is typically very low (for example, $FeNi_3$ and Cr_2Pt_3). Figure 2 shows similar plots for DS2.

In Ref. 1, ridge regression, kernel ridge regression, neural networks, and random-forest machine-learning methods were all tested and the random-forest model made the most accurate predictions. We used DS1 in a *k*-nearest neighbors model and compared its performance to the accuracy of the random-forest model. The *k*-NN algorithm was varied for 1–20 neighbors to determine the optimal *k*. A *k*-NN model with 2 neighbors provided best prediction accuracy but was not as good as the random forest (see Fig. 3).

To see how well the DS1 random-forest model generalizes on unseen data, we did a "blind" test on all the data in DS2 (see Fig. 4). 54% of the predicted Curie temperatures were within 50 K and 70% within 100 K. The mean absolute error was 90 K. This is a larger error than the prediction error using DS1 data; however, the model still makes relatively accurate predictions on around 2000 previously unseen magnets. We also used k-fold cross validation to show how the addition of DS2 data affects our predictive accuracy. 50 iterations of threefold cross validation show that DS1 averages an MAE of 73 K and a standard deviation of 3.2. A combination of DS1 and DS2 averages an MAE of 71 K and a standard deviation of 2.3.

While the random-forest results are encouraging, a few different strategies were tried to improve the random-forest predictions. One of these strategies is to reduce the number of dimensions in the DS1 design matrix. A random forest was made for a range (5–85) of features using principal component analysis (PCA). PCA is not helpful to our model because, although noisy, the change in mean absolute error for each dataset shows that the accuracy improves up to about 60 features and stops improving after that as already observed in Ref. 1.

Another improvement strategy is designing better features. The MAST-ML[38] Python library can generate descriptors based on about one hundred atomic properties (such as ionic radius and electronegativity). Using MAST-ML, we generated 428 features for the compounds in DS1 and selected the top 20 most meaningful ones identified through MAST-ML's `EnsembleModelFeatureSelector` method, which uses a random-forest model to rank feature importance. Figure 5 shows these features used in a random forest and the comparison between these predictions and our random-forest-model predictions in Fig. 3. The MAST-ML features yield practically the same accuracy as with the original features. This is somewhat surprising because the MAST-ML descriptors incorporate many atomic properties, not merely the composition. However, Ref. 39 shows that the domain knowledge in the generated features is not expected to improve prediction accuracy over simple fractional features when using large amounts of data. Our results suggest that DS1 is large enough to make an accurate model using our original fractional features. While the size of ML model using the MAST-ML descriptors is significantly smaller than the size of the model using the composition-only descriptors, both models have the same accuracy and both are efficient enough to be used in the large searches below. Our final models used the composition-only descriptors.

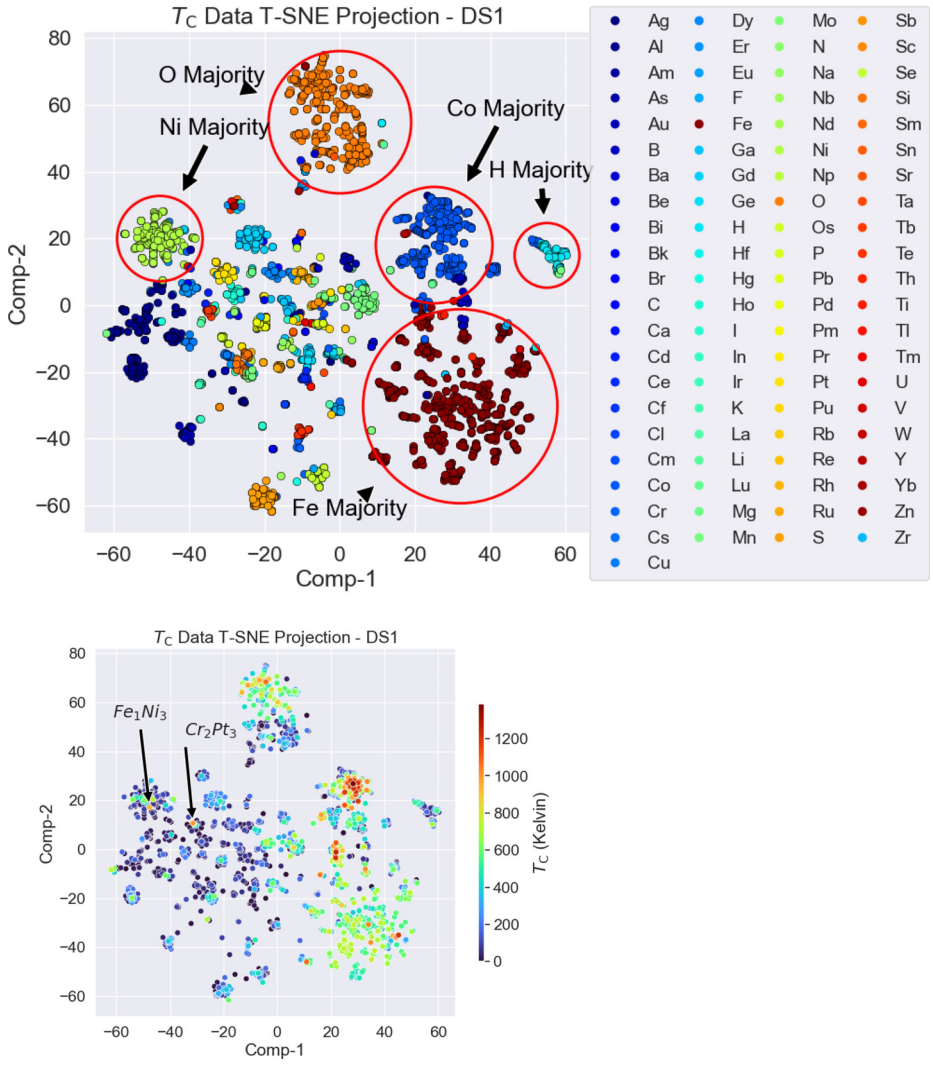
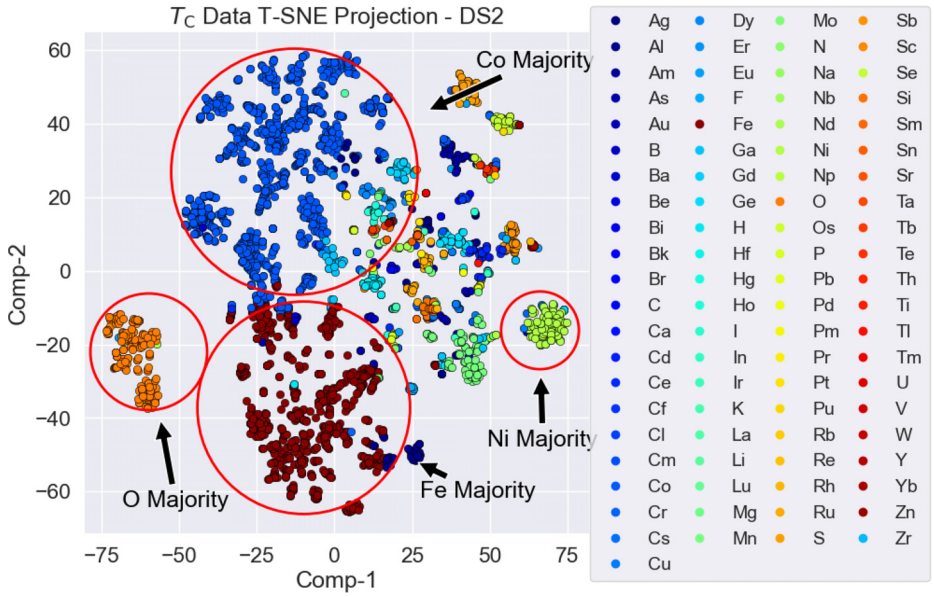


FIG. 1. (a) Experimental data (DS1) projected from the 85-dimensional feature space to two dimensions in a t-SNE[34] plot. Colors were assigned based on the majority element in each compound. (b) DS1 represented as a two-dimensional t-SNE plot. Colors were assigned based on the Curie temperature. Two compounds, Fe_1Ni_3 and Cr_2Pt_3, have anomalously high Curie temperatures, relative to others in the same cluster.

Getting more balanced training data may be another way to improve the model. An analysis of DS1 shows a significant imbalance, 38% of the magnetic materials have a T_C 0–100 K, while only 15% have a T_C 600–1400 K. This could lead the model to reduce the prediction error at low temperatures at the expense of making larger errors at high temperatures. This is counter to the purpose of the model, which is to discover candidate high-T_C magnets. Thus, we down-sampled the low-T_C compounds to more evenly distribute DS1. The resulting model is shown in Fig. 6. Even though there is a high density of low-T_C compounds, apparently they are necessary for accurate predictions of higher-T_C compounds. The balanced data predictions for high-T_C materials are not as good as with the original model, with an accuracy of 10% less within 50 K, 14% less within 100 K, and the mean absolute error 14 K higher.

Let us make one final comment before using the ML model to search for new high-T_C materials. With this unprecedented large database of magnetic compounds, a large range of training set sizes are possible so that the learning rate of the model can be estimated. Figure 7 shows the MAE on a test set of 850 compounds (approximately 1/3 the size of DS1, similar to the predictions in Fig. 3) while the training set is increased, using the remaining data. The process was repeated 100 times and averaged. A linear fit reveals a slope of ≈ -0.22. This learning rate is not particularly fast, but a better learning rate is probably not possible with composition-only descriptors. To reduce the MAE to 50 K in the current model, class would require a near tripling of the data.

The purpose of the ML model is to enable identification of candidate high-T_C materials. Our first attempt was to sweep over compositions of binary materials, but this revealed a systematic error. The error persists independent of the training data (DS1 or DS2), the particular ML method (random forest, k-NN), or the descriptors. Figure 8 compares the predictions with the experimental T_C of eight different sets of binary systems. The top four red subplots analyze four different high-T_C materials, and the four lower blue subplots analyze four different low-T_C materials. Each subplot shows the actual T_C value (red points) compared to the ML prediction (black line). A clear



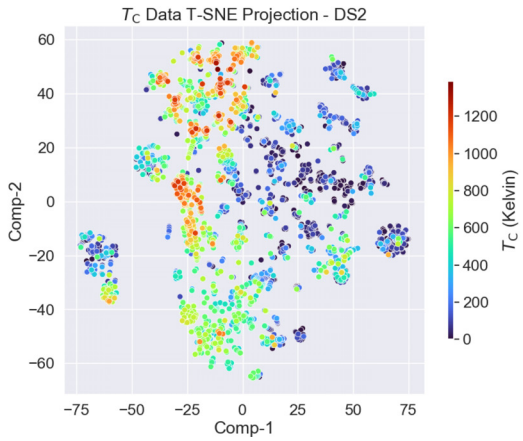


FIG. 2. (a) Experimental data (DS2) projected from the 85-dimensional feature space to two dimensions in a t-SNE[34] plot. Colors were assigned based on the majority element in each compound. (b) DS2 represented as a two-dimensional t-SNE plot. Colors were assigned based on the Curie temperature.

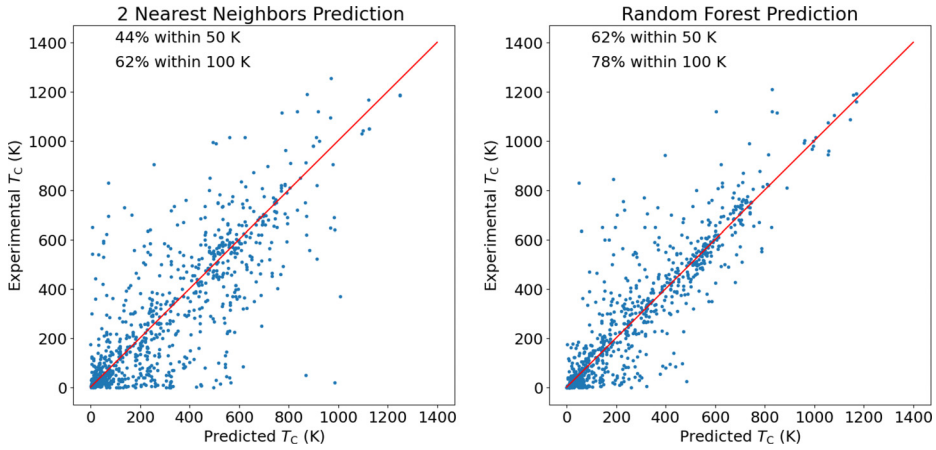


FIG. 3. *k*-nearest neighbor and random-forest predictions. (Left) prediction with the *k*-NN model with $k = 2$. 44% of the T_C predictions were within 50 K of the actual values and 64% were within 100 K. The mean absolute error was 109 K. (A 2-NN model with randomly shuffled T_C values gives a MAE of 270 K). (Right) random-forest prediction. 62% of the T_C predictions were within 50 K of the actual values and 78% were within 100 K. The mean absolute error was 69 K. (A random-forest model with randomly shuffled T_C values gives a MAE of 240 K.)

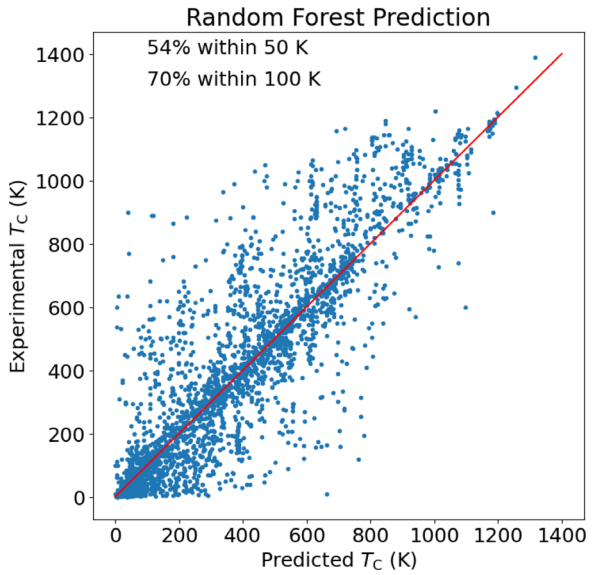


FIG. 4. Random-forest model trained on DS1 and validated with DS2. 54% of the T_C predictions for DS2 were within 50 K of the actual values and 70% were within 100 K. The mean absolute error was 90 K.

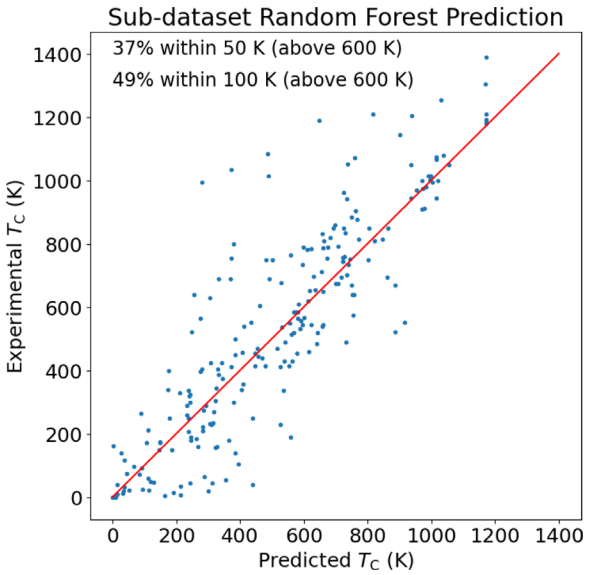


FIG. 6. Random-forest prediction with a balanced dataset. The Curie temperatures of the test data above 600 K were predicted with an accuracy of 37% of the data within 50 K and 49% within 100 K. The mean absolute error for those points was 141 K.

pattern emerges: between experimental data points, the ML model, instead of interpolating smoothly, drifts toward the average T_C of the training data (293 K). In the case of high-T_C materials, deep "valleys" occur in the absence of nearby experimental data. For low-T_C materials, the model tends to overestimate between training points. In a pattern reminiscent of Gaussian processes, the model tends to "regress toward the mean."

This systematic drift toward the mean can be seen across all the test data in Fig. 9 (left), which shows the difference between the predicted and the experimental T_C for the test data as a function of the experimental T_C (the random-forest model using DS1). Intuition suggests that this systematic error could be mitigated simply by shifting and re-scaling according to the black line in the figure. However, Fig. 9 (right) demonstrates that this does not work. The errors and the predicted T_C's are not correlated. The reader should remember that correlation is not transitive in general. Although the errors are correlated

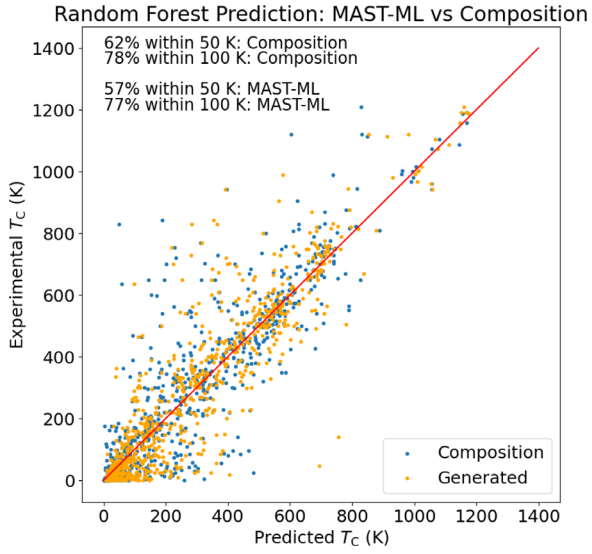


FIG. 5. Random-forest prediction using features based on the composition and 20 of the features generated by the MAST-ML[38] Python library. 62% of the T_C predictions for DS1 were within 50 K of the actual values, and 78% were within 100 K The mean absolute error was 69 K. 57% of the T_C predictions for the MAST-ML data were within 50 K of the actual values, and 77% were within 100 K. The mean absolute error was 70 K.

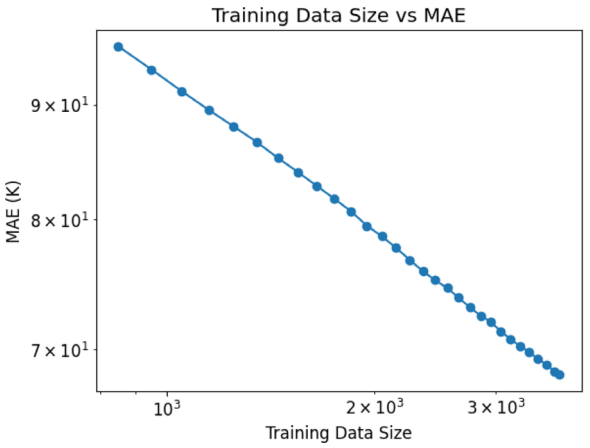


FIG. 7. MAE vs the amount of training data in a combined set of DS1 and DS2. For each iteration, the test data were a new random sample of 850 compounds while the training data were randomly sampled from the remaining data.

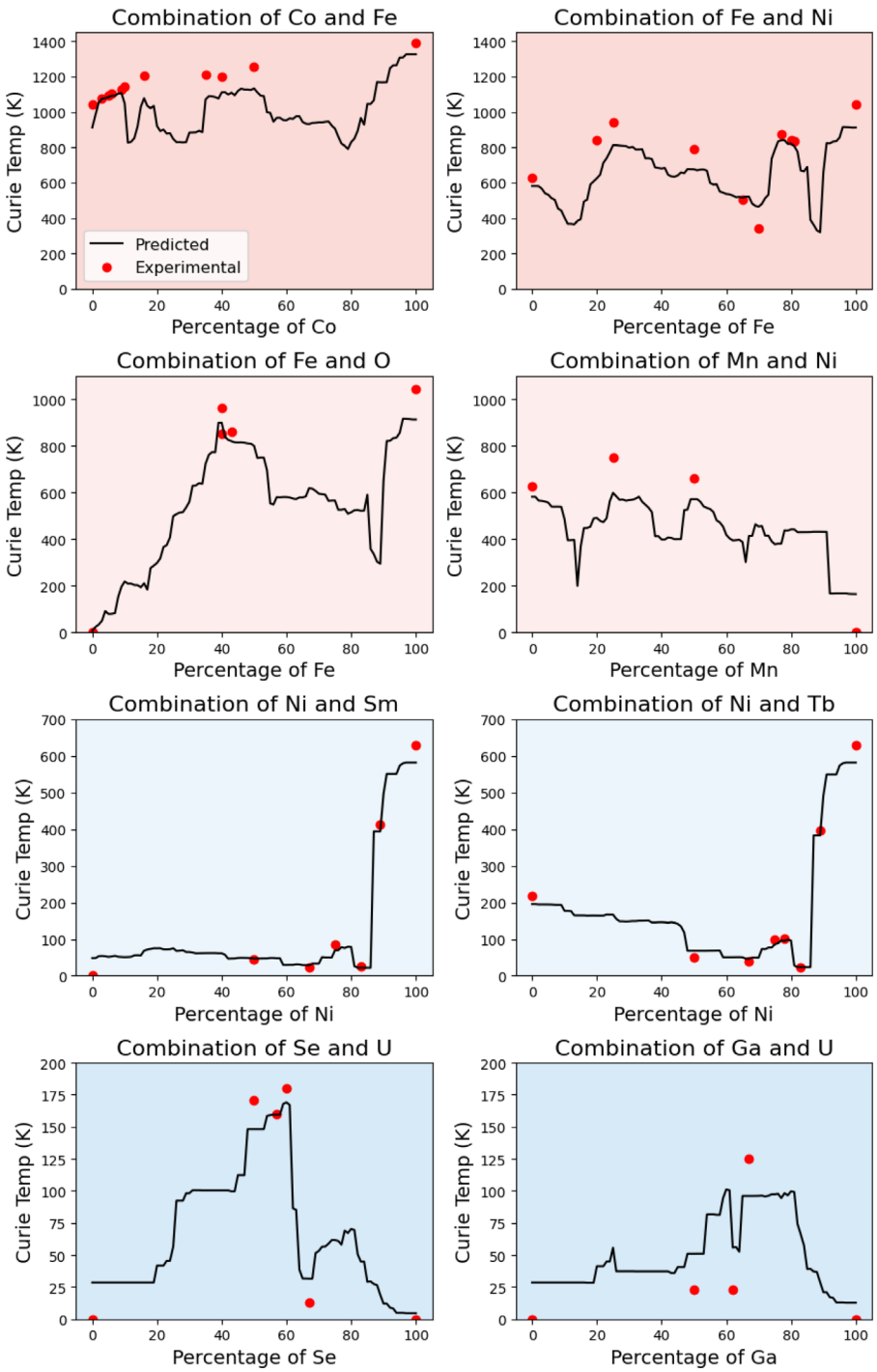


FIG. 8. Eight plots showing the Curie temperatures for eight different binary compounds. Horizontal rows share the same scale on the y axis. The black lines show the random-forest-predicted Curie temperatures across the entire composition range (step size: +1 at. %). The red dots are experimental data.

with the experimental T_C's and the experimental and predicted T_C's are correlated, the errors and the predicted T_C's are not necessarily correlated.

Recognizing the systematic error in predictions and being more interested in the accuracy of high-T_C predictions, we trained a random-forest model on a combined set of DS1 and DS2 but only included the 967 compounds with $T_C > 600$ K, thus boosting the mean of the training data from 293 to 825 K and mitigating the regression to the mean. Obviously this new model cannot be used to predict low-T_C materials but as we are primarily concerned with high-T_C

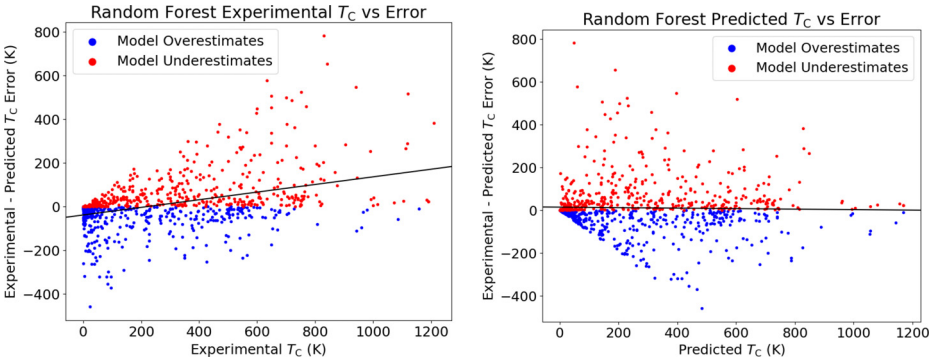


FIG. 9. Prediction error of the random-forest model (experimental minus prediction). (Left) error vs experimental T_C values. (Right) error vs predicted T_C values. The black line is the line of best fit. The errors are correlated with the experimental T_C but not with the predicted T_C.

materials, this new model with a higher average protects the predictions from straying too far in data-deficient areas.

This new high-T_C-only model was used to search composition space for all binary and ternary candidate compounds with exceptionally high-T_C's. The high-T_C-only model used only 71 features, restricted to elements that appear in compounds with $T_C > 600$ K. Figures 1 and 2 show that most of the highest-T_C compounds contain either cobalt, iron, or both. Using these elements, we generated every possible ternary combination containing iron, cobalt, and one of the other 69 elements (X_1) in 1% increments. The random-forest model can rapidly predict T_C for this entire set. Figure 10 displays the maximum predicted T_C of each combination of cobalt, iron, and X_1. While cobalt clearly dominates the high-T_C compounds, materials with a high iron concentration also are predicted to have a high T_C and are worth exploring because iron is much cheaper than cobalt.[41] Figure 11 shows similar predictions but for iron-rich ternary and binary candidates, which are inexpensive. These predictions suggest that, at least in general, for maximizing T_C, it is difficult to beat cobalt-rich materials, and that for minimizing materials cost for a relatively high T_C, iron-rich materials are difficult to beat. Other searches excluding cobalt and iron were also performed but no competitive materials emerged.

Unsuspected high-T_C materials sometimes appear. For example, see $FeNi_3$ and Cr_2Pt_3 in Fig. 1—these turn up in clusters with very low Curie temperatures. However, atomic structure, not merely composition, evidently plays an essential role in such materials. Devoid of explicit structure in the training data or the model, our predictions cannot be expected to include such candidates. Our models can learn a major portion of the relationship between chemical composition and Curie temperature and, thus, generally predict quite accurately. However, it seems that finding exceptional cases will require data that includes structural information and a model that incorporates explicit relationships between magnetism and structure. As discussed at the beginning, the reliability of such models remains challenging, and corresponding data are limited, so computational discovery of new high-T_C materials remains an outstanding challenge.

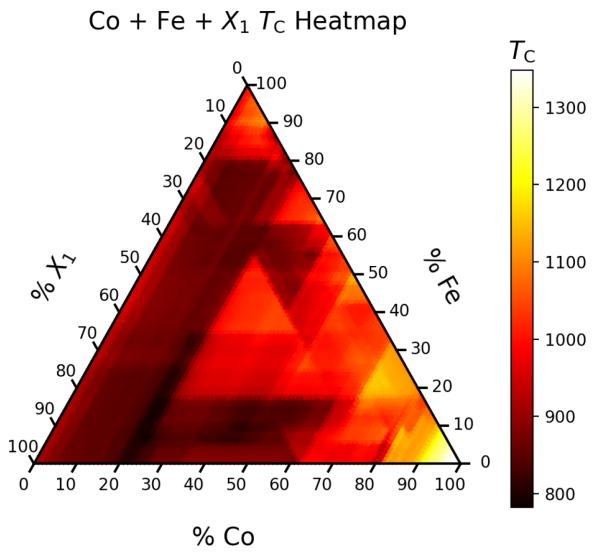


FIG. 10. Heat map showing the maximum predicted T_C of each combination of cobalt, iron, and X_1, where X_1 can be any element in materials with a T_C over 600 K found in DS1 and DS2 (excluding cobalt and iron). T_C is measured in Kelvins. Plot created using Python–Ternary.[40]

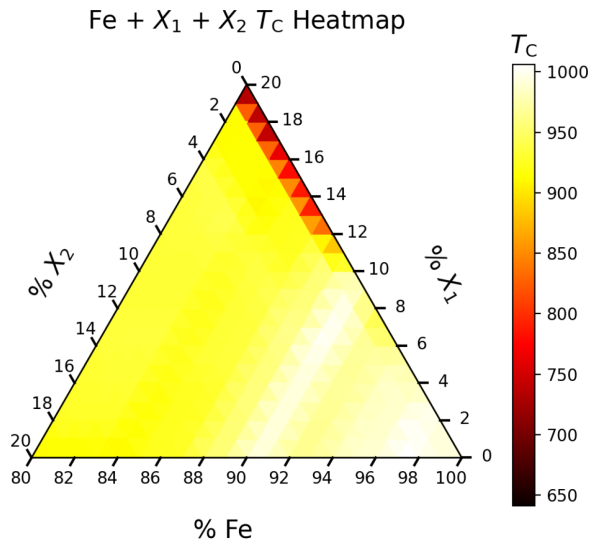


FIG. 11. Heat map showing the maximum predicted T_C of each combination of iron, X_1 and X_2 where X_1 and X_2 can be any element in materials with a T_C over 600 K found in DS1 and DS2 excluding cobalt and iron. Each compound is composed of a minimum of 80% iron. T_C is measured in Kelvins. Plot created using Python–Ternary.[40] (This plot should not be directly compared with Fig. 10 because of the difference in color scales.)

See the supplementary material for the details of two error plots from the 2-NN predictions shown in the left plot of Fig. 3, including a plot of the number of features reduced by PCA vs the MAE of the predictions made by a random-forest model using that number of features.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Joshua F. Belot: Conceptualization (equal); Formal analysis (lead); Funding acquisition (equal); Investigation (lead); Methodology (equal); Project administration (equal); Software (lead); Validation (lead); Visualization (lead); Writing – original draft (lead); Writing – review & editing (equal). **Valentin Taufour:** Conceptualization (equal); Data curation (lead); Funding acquisition (equal); Resources (equal); Supervision (equal); Writing – review & editing (equal). **Stefano Sanvito:** Conceptualization (equal); Data curation (lead); Funding acquisition (equal); Resources (equal); Supervision (supporting); Validation (supporting); Writing – review & editing (equal). **Gus Hart:** Conceptualization (lead); Formal analysis (equal); Funding acquisition (equal); Investigation (equal); Methodology (equal); Project administration (equal); Resources (equal); Supervision (equal); Visualization (supporting); Writing – original draft (supporting); Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are openly available in the ML-for-CurieTemp-Predictions repository at https://github.com/msg-byu/ML-for-CurieTemp-Predictions, Ref. 42.

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