Deep Learning Based Superconductivity Prediction and Experimental Tests

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Abstract

The discovery of novel superconducting materials is a longstanding challenge in materials science, with a wealth of potential for applications in energy, transportation, and computing. Recent advances in artificial intelligence (AI) have enabled expediting the search for new materials by efficiently utilizing vast materials databases. In this study, we developed an approach based on deep learning (DL) to predict new superconducting materials. We have synthesized a compound derived from our DL network and confirmed its superconducting properties in agreement with our prediction. Our approach is also compared to previous work based on random forests (RFs). In particular, RFs require knowledge of the chemical properties of the compound, while our neural net inputs depend solely on the chemical composition. We further discuss the existing limitations and challenges associated with using AI to predict and discover new superconductors, along with potential future research directions.

1 Introduction

Superconductivity is a phenomenon characterized by zero electrical resistivity and the Meissner effect – the diamagnetic expulsion of of magnetic fields from the bulk of the sample, and is microscopically attributed to the formation of Cooper pairs, making it an ideal system for the study of quantum entanglement [2, 14, 3]. The search for new superconducting materials has been a long-standing challenge in materials science with potential applications in energy, transportation, and computing [26, 35, 12]. Traditional methods of discovering new superconductors involve extensive experimental trial and error, which can be time-consuming and expensive. In recent years, researchers have explored the use of machine learning algorithms to accelerate the discovery of new materials [1, 21, 16, 24].

Modern machine learning techniques, such as deep learning [19], combined with genetic algorithms [10], can efficiently screen large databases of materials properties and predict the properties of potential new materials [30, 29, 34]. Beyond identifying potential materials, machine learning has also emerged as a tool for providing researchers with a deeper understanding of certain properties. For example, machine learning was used to develop simple models that explain the electronic structures of half-Heusler phases for potential thermoelectric properties [11], or direct the search for compounds with high hardness [23] by predicting the elastic moduli as a proxy [22], and so on.

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In this work, we evaluated the effectiveness of deep learning methods to classify materials into superconductor/non-superconductors and also to predict T_c when it is a superconductor. Our tools were applied to predict superconducting properties of hypothetical materials in sigma phases and compared to experimental findings. On this very special and small set of materials, the performance of both the random forest method and our deep learning networks are mixed. Still, we believe that we are at the beginning of the integration of AI and experimental synthesis, and this integration has immense potential for expediting the discovery of new superconductors and facilitating a deeper understanding of the underlying superconductivity phenomena. Previous works have used random forest regression [33], gradient boosting [15], or, in the realm of DNN (deep neural networks), a combination of a CNN and an LSTM for T_c prediction [20], a neural network for T_c prediction without classification [18], and a network with Deep Set architecture for classification [28]. Recently, superconductor design through gradient optimization [13] has been used. Our approach differs from these, as we present below. We also find superior performance to regression algorithms trained with chemical features. In the present work, we rely solely on the chemical formula of the compound.

2 Deep Learning Superconductivity Prediction

2.1 Data and Preprocessing

The superconducting data for alloys were retrieved from database for superconducting materials, SuperCon [25]. The data tabulates the experimental results of measurements of superconductivity for 16,414 compounds. Each row indicates the elements in the compound and their respective percentages (the input), as well as the measured T_c value (the output), where $T_c > 0$ indicates that the compound is superconducting.

For each data point, a data vector of length 120 is generated with the index representing the atomic number of elements and its corresponding percentage being the entry for that index. These generate 16,414 sparse 120-dimensional vectors. This will be the input of our fully connected network. In principle, it may be useful to incorporate some information about the relative position of elements in the periodic table. Several works [18, 13] break up the periodic table into multiple rectangles and input the chemical compound as multiple images which is then processed by a convolutional network (CNN). We will reshape the 120 dimensional vector into a single 10×12 'image'. This approach is harder to justify, a priori, but, as we will see, our CNN seems to have slightly better performance in some cases, compared to the fully-connected network. We speculate that it benefits from bringing together chemicallly similar elements.

The output comprises two components: classification ground truth, represented by a single binary value of 0 or 1, indicating the presence or absence of superconductivity. Thus, the two classes correspond to non-superconducting compounds (0) and superconducting compounds (1). The other component is the measured T_c value.

2.2 Architecture

Given the nature of the dataset, we decided to treat the problem as a combination of classification and regression tasks. In other words, we construct deep neural nets (DNNs) that can classify whether a given compound is superconductive or not and predict the corresponding T_c value. The DNN model comprises three components: the network backbone and two prediction branches: one for classification and the other for T_c value. The architecture is schematically illustrated in Fig. 1, left. We build two networks, one fully-connected, the other convolutional. For the details of the architectures, please see Supplementary Materials. The DNN model is implemented using the PyTorch [27] framework, which accepts network data in the 4-D tensor format of NCDHW (batch N, channels C, depth D, height H, width W).

A word of justification for our choice of the branched architecture and on our planned method of training. Since the two tasks, namely, the classification of superconducting nature and the regression of T_c are related, it makes sense to train a set of shared latent variables as neurons in the initial layers. Since the teaching signal from T_c is more specific than the signal from the class, we train the shared part via the regression task. Since the classification task is conceptionally easier than the regression task, we choose to allow some additional flexibility to the network, rather than restricting

to it classifiers obtained by thresholding the output of a regression network, as in Refs. [33, 18] and others.

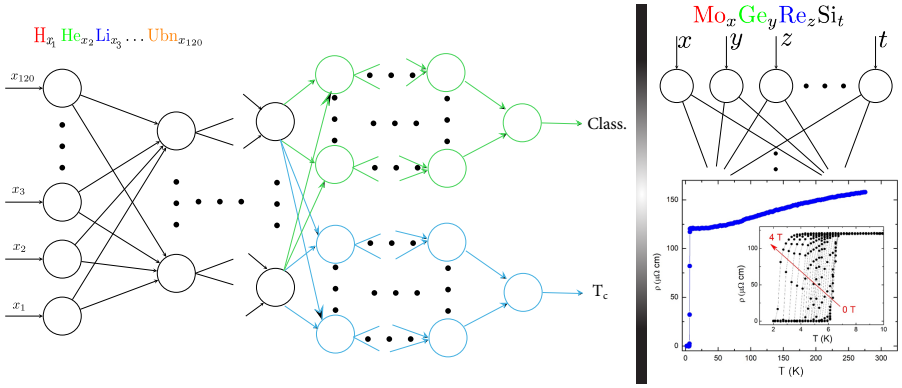

Figure 1: Left: DNN structure with a shared backbone and two prediction branches, one for the T_c value and the other for classification. We have used our DNN to predict a new superconductor (see Sec. 3) from the σ family of alloys, and measured its resistivity as a function of temperature, extracting T_c.

2.3 Training

The data set is divided into 2 portions: training (13132 entries) and testing dataset (3282 entries). During the training process, the Mean Squared Error (MSE) is utilized to compute the loss error, which is subsequently leveraged for the backpropagation calculation using the Adam optimizer [17]. The training process is carried out in two stages. First, the Backbone and T_c prediction branches are jointly trained, and the loss of the predicted T_c value versus the ground truth is used for network backpropagation. Once the T_c Prediction results reach a satisfactory level, the parameters of the Backbone and T_c Prediction branches are fixed. The training is then performed solely on the Classification branch. Each branch was run for 5,000 epochs. This procedure was performed for both architectures. The learning curves, showcasing performance in accuracy and MSE loss are plotted in Fig. 2

After completing Stage1 and Stage2 training, the model is finalized for testing. The training process is further optimized by using two-step learning rate decay. The initial learning rate is set to 0.0001, and at 3000 epochs, it is decayed to 0.00001 to fine-tune the training parameters. The training results are evaluated based on the backbone and T_c prediction branch training, and the T_c prediction difference is calculated by averaging the mean absolute error (MAE) difference between the predicted and ground-truth values [8]. A lower difference value indicates more accurate prediction results. Both the loss and T_c prediction differences decrease with an increase in epoch count, and starting from

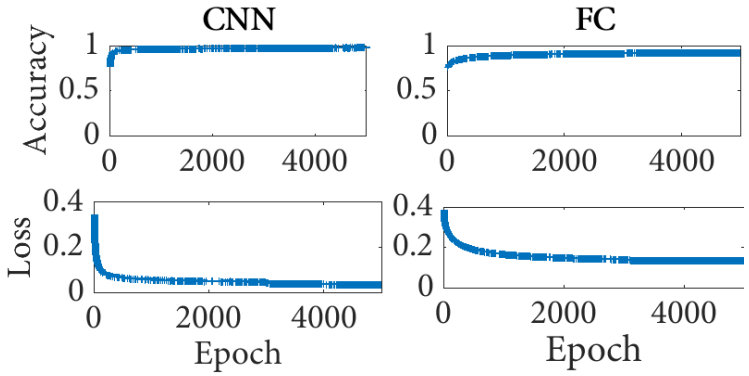

Figure 2: Performance against epochs of training for the CNN (convolutional neural network) and FC (fully-connected neural network). See main text for details.

the 2000th epoch, the loss and difference curve reach a plateau. However, at the 3000th epoch, with a decay in the learning rate from 0.0001 to 0.00001, the loss and T_c prediction differences further decrease, indicating that the learning rate decay indeed helps to improve the training process by providing finer granularity control of parameter updating.

2.4 Results

Results and the performance of the classification branch is evaluated based on its accuracy in correctly identifying if a compound exhibits superconductivity or not, as compared to the ground-truth. A higher accuracy value indicates better performance in the classification task. The testing process involves evaluating the performance of the trained model on a separate dataset known as the test dataset, which is distinct from the data used during model training. The test dataset comprises a total of 3282 entries. The final training and testing results with appropriate comparison to random forest methods are listed in Table 1.

Table 1: The summary of classification and regression test results for various methods. RF= Random Forest [33], FCNN= Fully-connected neural net, CNN= Convolutional Neural Net. The error in T_c regression (Reg.) is defined as the mean of $T_c(\text{pred.}) - T_c(\text{actual})$.

Model	Accuracy	Precision	Recall	F1	Reg. [K]	Class.
RF [33]	85% [1]	85%	94%	90%	7.88 ± 0.52	NA [2]
FCNN	83 ± 0.6 %	85 ± 0.7%	**95 ± 0.4%**	90%	4.497 ± 0.328	83.04 ± 0.6%
CNN	85 ± 0.3%	**88 ± 0.4%**	92 ± 0.3%	90%	**3.208 ± 0.180**	**84.77 ± 0.3%**

The SuperCon database [25] has 16,414 entries, 12,499 ($\approx 76\%$) of which are known to be superconductors and the rest are considered non-superconducting. Note that a positive/negative weight guessing random classifier could achieve a maximum of $\approx 76\%$ accuracy by always going with the majority class [4]. In this dataset, the majority class predictor would have 100% recall but $\approx 76\%$ precision. These baselines are to be compared with the classification performances of the machine learning methods.

3 Experimental Studies

Superconductivity was observed in a few materials belonging to the σ-phase category [6], characterized by a high degree of disorder and the presence of multiple elements occupying the same Wyckoff position. The occurrence of σ-phases is strongly dependent on the concentration and the type of the constituent elements. Notably, superconductivity has been demonstrated in materials such as Nb-Ru-Ge, Nb-Rh-Ge, and Nb-Rh-Si, which has stimulated further investigations into Re-based materials with varying ternary systems to explore the their superconducting properties [5, 7].

We leveraged our chemical intuition and expertise, to narrow our search for new superconductors to ternary compounds with formula unit $Mo_{20}X_6Z_4$, with X=Re, Rh, Ru, Z=Ge, Si, as the 20-6-4 stoichiometry is most likely to form in the sigma phase. Then we use our DNN-based algorithm to investigate the potential superconducting properties of these compounds. Our CNN predicted that **Mo_4Re_2Si** is likely to exhibit superconductivity with a critical temperature (T_c) of approximately 6 K, while **Mo_4Re_2Ge** is also predicted to be a superconductor with $T_c \sim 5$ K. The drop in resistivity for the associated, fully stoichiometric compound of the $20-6-4$ family, **$Mo_{20}Re_6Si_4$**, is shown in Fig. 1(right). Subsection A.4 provides further details of the experimental set up, synthesis, crystal structure and additional measurements performed to confirm the 3D nature of the superconductivity.

Data leakage related issues are discussed in subsection A.3. For clarity, by starting with the loading composition of 4-2-1 ratio, we get final products with around 20-6-4 ratio.

[1] To match with our definition of accuracy, this value was extrapolated from Stanev *et al.* to the point $T_{sep} = 0$.

[2] Stanev *et al.* do not explicity train for classification, we do not present a direct comparison as it would be fine-tuned by their value of T_{sep}.

4 Conclusion

This work proposes a DNN-based superconductivity prediction model that uses 13132 data points to achieve an accuracy of 84% on 3282 test data. This is a small dataset compared to many cutting edge applications of DNNs. For instance, popular image classification algorithms such as mobile-net and res-net that use ImageNet as a basis for training are trained on 1.2 million images to classify 1000 objects. The top-1 accuracy for ImageNet has moved into 90% plus territory only within the last few years (see `https://paperswithcode.com/sota/image-classification-on-imagenet`). Our performance is comparable to previous work using random forests, but does not require detailed atomic-level chemical information utilized by Stanev et al. [33] while using random forests. Unlike Konno *et al.* [18] and Pereti *et al.* [28], our dataset contains only real compounds extracted from SuperCon, without padding with fictitious entries for increased sensitivity. Our data is further not restricted to the high-T_c regime as in Ref. [13], but is composed of data for a wide range of superconducting temperatures. In classification we find comparable performance relative to a more involved algorithm as in Ref. [28].

5 Limitations of This Study and Future Directions

We train our model on a relatively small dataset with an abundance of superconductors. To enhance the prediction accuracy and robustness of the model, more training data, with appropriate materials distribution, is required. More importantly, the input in our dataset only contains the chemical composition of the material. One extension is to encode the neighborhood of elements in the periodic table, as in the graph sometimes known as the “periodic spiral" [31]. The sigma phase experiments indicate that all the methods have difficulties differentiating between elements in the same group. Utilizing the crystal structure [32] and electronic structure can provide additional information to the model to abstract during the training process. Also interesting is the use of symmetries for prediction [36].

These augmentations of predictors could boost the model’s performance and make predictions in real-world scenarios.

6 Acknowledgements

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7 Data Availability

The original SuperCon data used in this study are available at the references given in this paper [25]. Datasets generated during the current study are available from the corresponding author on reasonable request. The code used in this work is freely available at: `https://github.com/danielkaplan137/TcMLPred.git`

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A Appendix / supplemental material

A.1 Details of Architecture

The convolutional model uses both convolution and pooling with the later stages being fully connected. The fully-connected model obviously uses all to all connections at every layer. The activation function used for both network is ReLU. We provide the visualization of the networks using the Netron software (`https://netron.app/`), based on the saved .onnx files.

A.2 Detailed plots of network performance during training/testing

Below, we present more expansive plots of the training process for accuracy and MSE loss in the two networks as a function of epoch.

A.3 Data leakage

We discuss the possible impact of data leakage [9] on our predictive power. Data leakage happens when the training data contains some kind of information that will not be available when the model is used for prediction or decision making. Such leakage has two main types:target leakage and train-test contamination. Target leakage occurs when training predictors include data that will not be available at the time to make new predictions. That is not relevant for us. As to test-train contamination, there was nothing in our dataset of the form $Mo_xRe_ySi_z$.

If one broadens the definition and considers similar materials, our dataset indeed has materials which share two of the three elements present in the target. While these materials, present in the dataset could be similar, for example, some materials of the form $Mo_xRe_yO_z$, superconductivity is dependent on many subtle effects and is not easy to predict. In fact, different compositions of $Mo_xRe_yO_z$ have different behavior. Also, while we are trying to predict new materials, we expect there are one or more chemical composition-wise similar superconducting materials. Thus, for computationally accessible new superconducting materials, some similarity in the data is expected.

A.4 Details of the experiment

$Mo_{20}Re_6Si_4$ was synthesized successfully by arc melting method, and its crystal structure was confirmed to be tetragonal with lattice parameters $a = b = 9.472(1)$ Å and $c = 4.965(2)$ Å. The compound belongs to the σ-phase, which has a large unit cell with 30 atoms and a general stoichiometry of $A_{20}B_{10}$ shown in Figure 9a. In binary σ-phases, A and B atoms occupy different Wyckoff positions, and in ternary σ-phases, the third element partially occupies some positions from A and/or B atoms. Although further experiments are required to determine all mixing and site occupancies, assuming the stoichiometry of $Mo_{20}Re_6Si_4$ can be used in further physical properties analysis.

Figure 9b displays the temperature dependence of the zero-field-cooled (ZFC) and field-cooled (FC) volume magnetic susceptibility measured under an applied magnetic field of 20 Oe. The transition to the superconducting state is observed at $T_c = 5.4$ K and was determined as the point of intersection between the steepest slope of χ_v and the extrapolation of the normal state susceptibility. This method is consistent with previous studies. The ZFC volume magnetic susceptibility slightly exceeds $4\pi\chi_v$ = -1, which is the expected value for a perfect Meissner effect. insights into the magnetic properties of the sample and are important for understanding the superconducting behavior of the material.

In order to gain a deeper understanding of the superconducting state of the material, we conducted resistivity measurements. The temperature dependence of the resistivity is depicted in Figure 9c. We observed a decrease in resistivity as the temperature increased, which is typical for metallic behavior. However, the resistivity values were found to be high, likely due to the high level of disorder present in the material. Notably, a sharp drop to zero resistivity was observed at a temperature of approximately 6 K, which is indicative of the superconducting transition.

Finally, to establish the bulk nature of the observed superconductivity, we performed specific heat measurements. The temperature dependence of C/T is presented in Figure 9d. We observed a λ-shaped anomaly, which indicates the presence of a phase transition. To identify the specific heat jump (ΔC) and critical temperature Tc, we constructed an equal-area entropy plot (red lines in the main panel of Figure 9d). The obtained Tc was determined to be 5.4 K, which is in agreement with the magnetic susceptibility data.

A.5 Computational Resources

All networks were trained on a 2 NVIDIA GPU compute nodes managed by the SUN Grid engine, on the Beowulf cluster, Rutgers university. 6 realization of each network were carried out, with the dataset sizes for training enumerated in the main text.

13132 training entries over 5000 epochs required 6 hours and 45 minutes for training for CNN networks and 6 hours and 50 minutes for FC networks. Testing on existing models was completed in 45 seconds (~ 3282 entries).

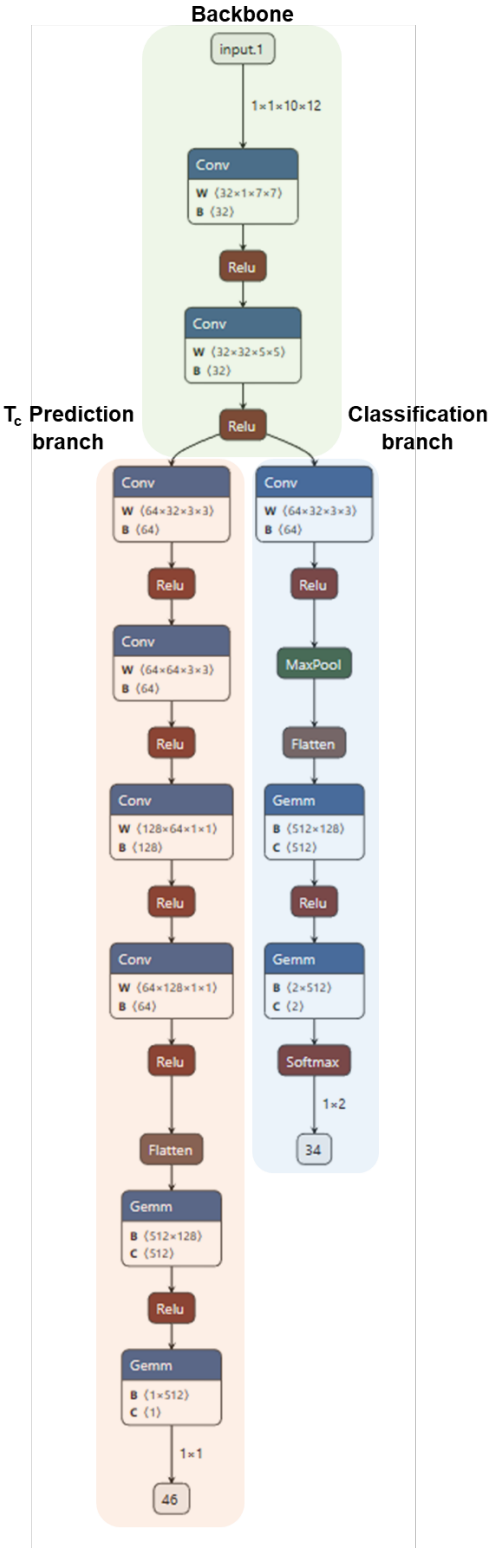

Figure 3: The convolutional model, including (1) Backbone, (2) T_c Prediction branch and (3) Classification branch.

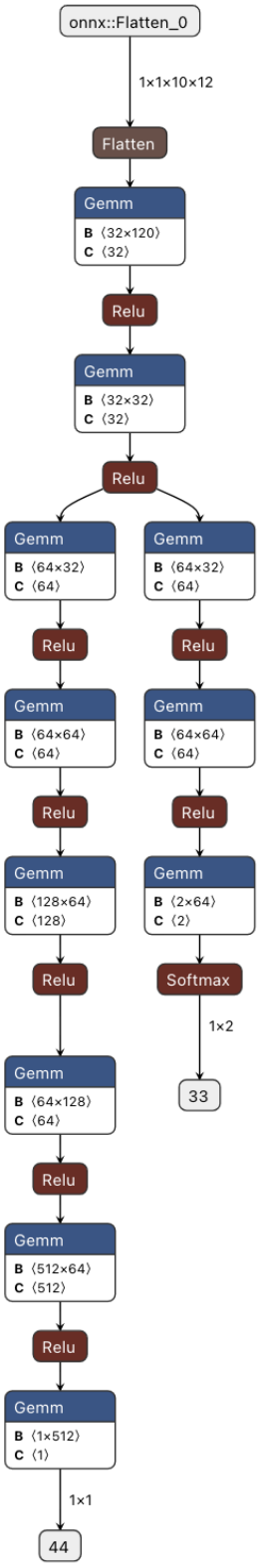

Figure 4: The fully-connected model.

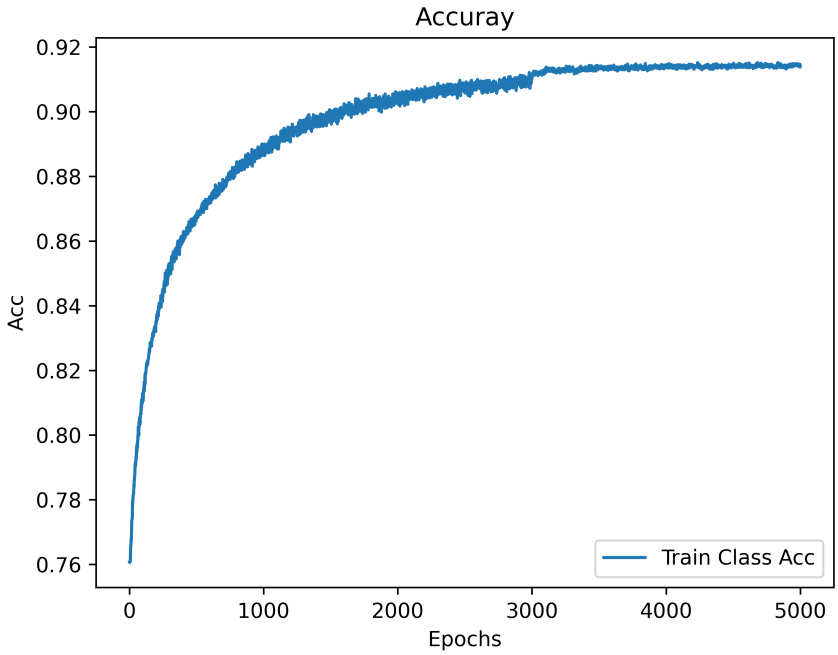

Figure 5: Fully-connected Model: Accuracy in classification during training with epoch.

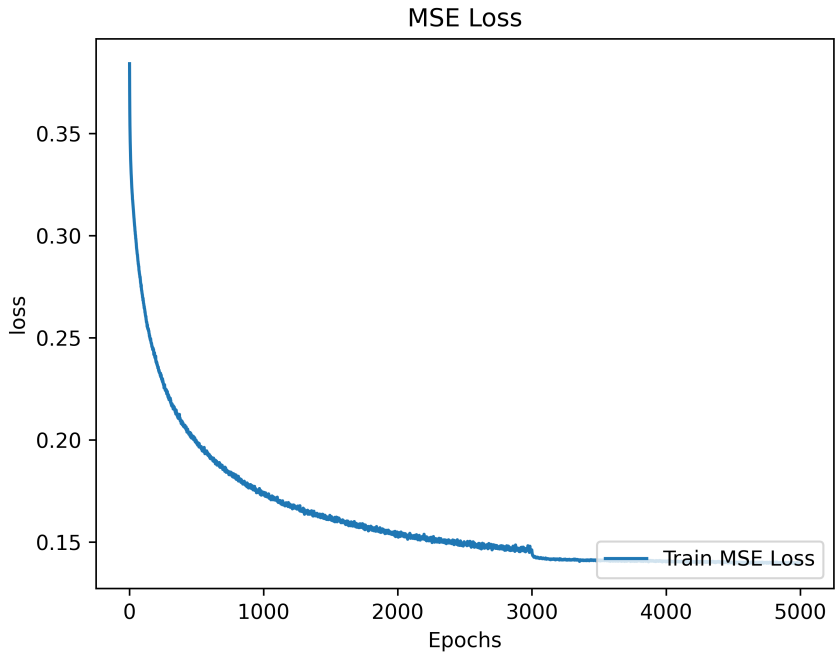

Figure 6: Fully-connected Model: MSE loss in classification during training.

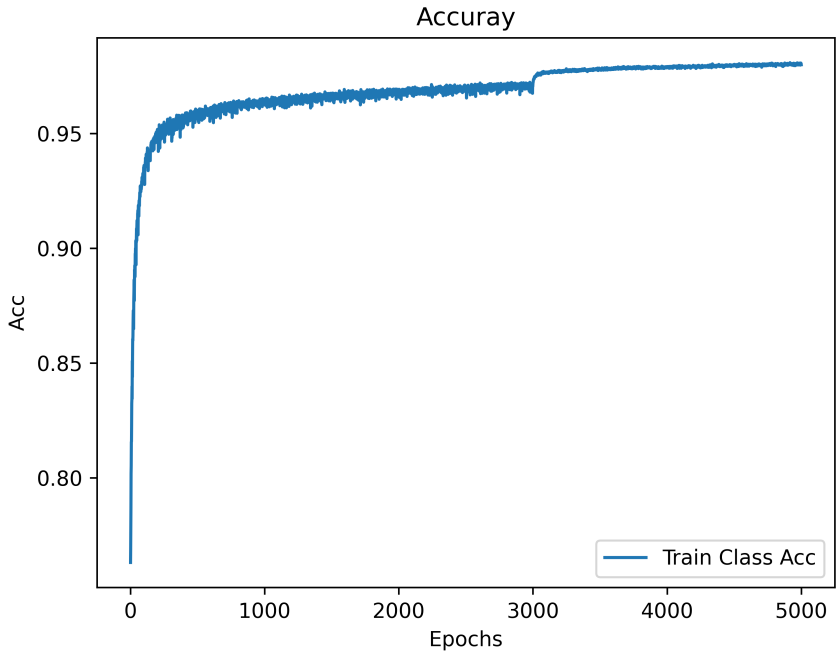

Figure 7: Convolutional Model: Accuracy in classification during training with epoch.

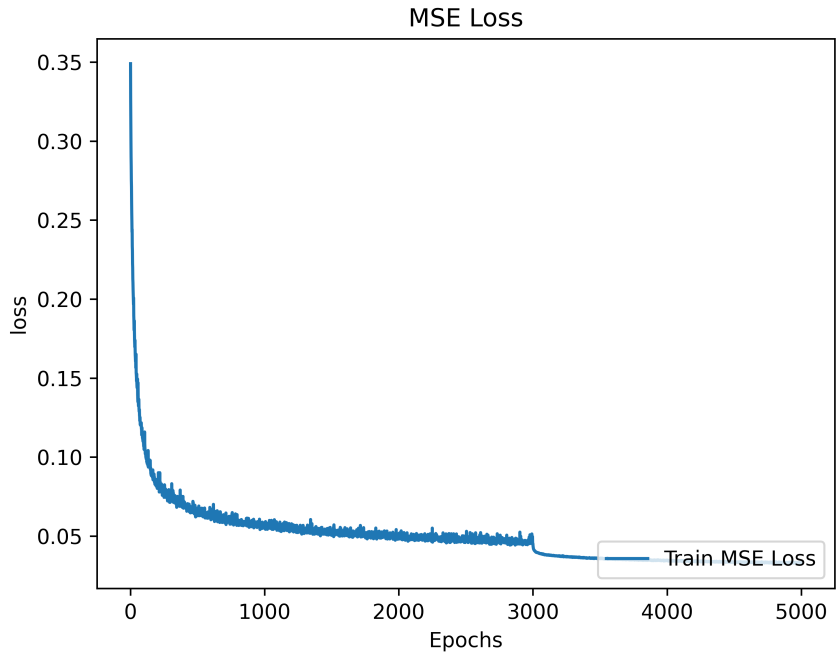

Figure 8: Convolutional Model: MSE loss in classification during training with epoch.

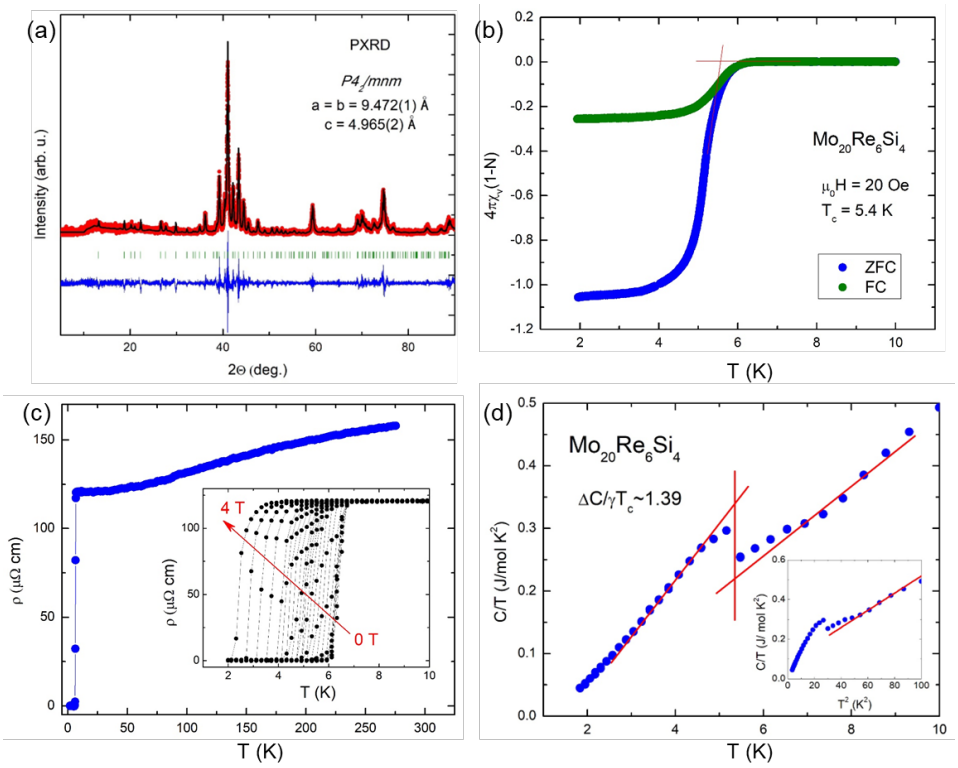

Figure 9: Phase identification and superconductivity properties of $Mo_{20}Re_6Si_4$. (a) Powder X-ray diffraction pattern of sigma phase $Mo_{20}Re_6Si_4$; (b) Magnetic susceptibility of $Mo_{20}Re_6Si_4$. (c) Field-dependent resistivity of $Mo_{20}Re_6Si_4$. (d) Heat capacity of $Mo_{20}Re_6Si_4$.

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