Predicting Superconductors' Critical Temperature Using Machine Learning: An Interdisciplinary Approach Combining Physics, Chemistry, and AI

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Superconductors, materials that exhibit zero electrical resistance below a critical temperature (Tc), are widely regarded as a cornerstone for future technologies including quantum computing, sustainable energy grids, and frictionless transportation systems. However, the discovery of new superconductors has historically been slow, limited by experimental cost and the challenges of theoretical prediction. This paper presents an interdisciplinary framework that integrates principles from physics and chemistry with modern machine learning methods to accelerate superconductor discovery. Using a dataset of over 21,000 materials, we engineered chemically informed features and trained a deep neural network to predict Tc with high accuracy (MAE ≈ 5K, RMSE ≈ 9K, R^2 ≈ 0.92). Beyond performance, our approach interprets model behavior through the lens of BCS theory, bridging data-driven insights with physical mechanisms. The societal potential of this work lies in its ability to reduce barriers to innovation, offering a scalable path toward materials that can enable cleaner energy transmission and more accessible advanced technologies. We also consider the challenges of relying on data-driven discovery in critical fields, underscoring the need for responsible and equitable development of AI-driven materials research.

Keywords: *superconductors; machine learning; computational materials science; responsible innovation*

LLMs were used in the writing process of this article.

1 Introduction

Superconductivity—the ability of a material to conduct electric current with zero resistance below a specific threshold temperature known as the critical temperature (Tc)—represents one of the most remarkable quantum phenomena in condensed matter physics. Since its discovery by Heike Kamerlingh Onnes in 1911, superconductivity has inspired generations of scientists due to its vast potential in real-world applications. From frictionless

maglev trains and MRI machines to quantum computers and lossless power grids, superconductors hold the promise of revolutionizing modern technology. Yet, despite over a century of research, the path toward identifying new superconductors—especially those with high critical temperatures—remains slow and empirical.

A key challenge in superconductor research is the accurate prediction of Tc. Traditional discovery methods involve extensive trial-and-error experimentation, which is costly, time-consuming, and often ineffective, particularly as the chemical complexity of materials increases. Even with the advancement of quantum mechanical models—such as BCS theory for conventional superconductors and Eliashberg theory for strong-coupling cases—Tc prediction remains a difficult problem. These models typically require intricate, material-specific inputs such as phonon spectra, electron-phonon coupling constants, and density of states, which are often unavailable or computationally expensive to derive.

Complicating matters further, unconventional superconductors—such as cuprates and iron-based materials—do not conform to the predictions of classical theories. In these systems, superconductivity emerges from mechanisms beyond phonon mediation, making Tc even harder to estimate from first principles. Moreover, given the enormous chemical space of potential superconducting compounds (estimated to be in the tens of millions), it is impractical to explore them all experimentally or theoretically.

Artificial Intelligence (AI), particularly machine learning (ML), offers a powerful new paradigm to address this challenge. ML models can learn complex, non-linear relationships directly from data, bypassing the need for explicit equations or assumptions. When applied to materials science—a field now undergoing a data revolution—ML enables rapid property prediction, inverse materials design, and intelligent screening across vast compositional landscapes. For superconductors, this means we can now attempt to predict Tc directly from a material's chemical composition using large datasets and modern deep learning architectures.

In this work, we present an interdisciplinary framework that integrates physics, chemistry, and machine learning to predict the critical temperature of superconducting materials. Leveraging a real-world dataset of over 21,000 superconductors sourced from the NIMS SuperCon database and curated by UCI, we extract numerical features from the chemical composition of each compound—ranging from atomic mass and electronegativity to thermal conductivity and valence electron counts. We then train a deep neural network (DNN), built using TensorFlow and Keras, to regress the critical temperature based on these features.

Our results show that the model not only generalizes well across both cuprate and non-cuprate superconductors but also achieves high accuracy, with a mean absolute error

(MAE) of ~5 K and an R2 score of ~0.92 on held-out test data. Furthermore, we interpret key features learned by the model and connect them back to physical principles such as Cooper pair formation, electron-lattice interactions, and density of states, demonstrating that data-driven models can retain physical relevance when properly structured.

Ultimately, this study demonstrates that machine learning is not merely a computational shortcut, but a complementary scientific tool that can augment theory, accelerate materials discovery, and guide experimental synthesis. By combining the interpretability of physics with the flexibility of AI, we open a new pathway toward the rational design of superconductors in the 21st century.

2 Data

The foundation of this study lies in a high-quality, real-world dataset consisting of over 21,000 superconducting materials and their corresponding critical temperatures (Tc). This dataset was obtained from the SuperCon database, a comprehensive resource curated by the National Institute for Materials Science (NIMS), Japan, and pre-processed by Kam Hamidieh (2018) for the UCI Machine Learning Repository. The dataset captures a wide diversity of superconductor families, including cuprates, iron-based, and conventional (low-Tc) materials.

2.1 Composition and Diversity

Each entry in the dataset consists of a chemical formula, its experimentally measured critical temperature in Kelvin, and 81 hand-crafted features derived from elemental composition that capture stoichiometric attributes, electronic properties, atomic properties, thermal and mechanical descriptors, and periodic table–based statistical measures, enabling machine learning models to learn relationships between elemental combinations and superconducting behavior without requiring detailed knowledge of crystal structure or electronic band diagrams.

2.2 Cuprate vs. non-Cuprate Classes

To better capture variation in superconducting mechanisms, we also categorized the dataset into two major superconductor classes:

- CSC (Cuprate-based Superconductors): Known for their layered structures and high Tc values (often >77 K, the boiling point of liquid nitrogen), cuprates form a significant part of high-Tc superconductor research.

- NCSC (Non-Cuprate Superconductors): This category includes both conventional low-Tc superconductors (e.g., NbTi, Pb, Hg) governed by phonon-mediated BCS theory, as well as emerging families like iron-based superconductors and heavy fermion systems.

3 Data Preprocessing

Before feeding the data into our machine learning pipeline, we applied the following preprocessing steps:

- Missing values: Rows with missing critical temperatures or invalid chemical formulas were removed.
- Feature scaling: All input features were standardized using a power transformation to ensure Gaussian-like distributions and improve neural network training stability.
- Train-test split: The dataset was split into 80% training and 20% test subsets, ensuring both sets retained proportional representation of cuprate and non-cuprate classes.
- Target transformation (optional): We experimented with applying a log-transformation to Tc values to reduce skewness but found that the raw target values yielded better results for our regression model.

This dataset provides an exceptional opportunity to train predictive models on a large, chemically diverse set of superconductors. It captures essential compositional information while being scalable, reproducible, and accessible—perfect for applying machine learning in a physically meaningful way.

4 Methods

In this section, we describe the theoretical foundations and computational strategies employed to predict the critical temperature Tc of superconductors. Our approach integrates insights from established superconductivity theory with a data-driven machine learning framework that learns patterns from chemical composition features. This hybrid method ensures both physical interpretability and predictive accuracy.

4.1 Physical Theory: BCS and Eliashberg Framework

At the microscopic level, superconductivity arises when electrons form bound states called Cooper pairs, mediated by interactions with lattice vibrations (phonons). According to Bardeen–Cooper–Schrieffer (BCS) theory, such pairing leads to a quantum mechanical ground state with zero electrical resistance below a material-specific critical temperature TcT_cTc.

For conventional superconductors (e.g., elemental metals and alloys), the BCS approximation gives:

$T_c \approx 1.13\theta_D \exp\left(-\frac{1}{N(0)V}\right)$

Where θ_D is the Debye temperature, representing phonon spectrum cut-off, N(0) is the electronic density of states at the Fermi level, and V is the effective attractive interaction between electrons.

However, for more accurate modelling—especially in strong-coupling superconductors—BCS theory is extended by Eliashberg theory, which includes retardation effects and uses the electron-phonon spectral function α2F(ω)\alpha^2F(\omega)α2F(ω). An empirical formula from Eliashberg formalism is the McMillan equation, modified by Allen and Dynes:

$T_c = \frac{\omega}{1.2} \exp\left(-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1.602\lambda)}\right)$

Where ω is the logarithmic average of phonon frequencies, λ is the electron-phonon coupling constant, and μ* is the Coulomb pseudopotential.

These formulas underscore that Tc depends on a complex interplay of lattice dynamics, electronic structure, and electron interactions, parameters often inaccessible from chemical formulas alone. Hence, we turn to machine learning, enabling us to extract predictive patterns from high-dimensional, compositional data without solving complex many-body physics directly.

4.2 Machine Learning Model: Deep Neural Network for Tc Prediction

4.2.1 Problem Framing

We cast Tc prediction as a supervised regression problem, where the input is an 81-dimensional feature vector derived from a compound's chemical composition, and the output is a real-valued scalar T_c. Formally:

$f(x)=T_c$

Where, $x \in R^{81}$ is the feature vector of elemental and statistical descriptors and f is the function learned by the neural network model.

4.2.2 Feature Engineering

The 81 features used in this study were extracted through domain-informed aggregations of elemental properties. Specifically, we calculated the mean, range, and standard deviation for key descriptors such as atomic mass, electronegativity, valence electron count, first ionization

energy, atomic radius, thermal conductivity, and electron affinity, among others. These features were deliberately selected to reflect physicochemical properties that directly influence superconducting behavior. For example, electron-lattice coupling is shaped by atomic mass and electronegativity, the electronic density of states is tied to valence electron counts, and phonon spectra are affected by both atomic radius and bonding strength. Together, these descriptors provided a chemically and physically meaningful basis for training the machine learning model.

4.2.3 Neural Network Architecture

We implemented a feedforward deep neural network (DNN) using the TensorFlow 2.0 and Keras libraries, tuning the architecture to maximize performance while incorporating strategies for regularization. The input layer contained 81 neurons corresponding to the engineered features. Three hidden layers were employed, consisting of 256, 128, and 64 neurons respectively, each with ReLU activation. The output layer consisted of a single neuron with linear activation to support regression. To prevent overfitting, we introduced dropout (0.3) after each hidden layer, applied batch normalization, and included L2 weight regularization with $\lambda = 0.001$. The model was optimized using Adam with a learning rate of 0.001, and training was performed with mean squared error (MSE) as the loss function. Early stopping was applied when validation loss plateaued, and training proceeded for up to 200 epochs with a batch size of 64. The implementation relied on TensorFlow 2.0 and Keras, along with Scikit-learn, Pandas, and NumPy for data preprocessing, feature scaling, and evaluation.

4.2.4 Training Strategy

The dataset was divided into three subsets to enable training, validation, and testing. Eighty percent of the data (approximately 17,000 compounds) was allocated to the training set, while 20% (about 4,200 compounds) was reserved for testing. Within the training data, a 10% validation split was applied and used for early stopping during model training. Preprocessing steps included feature standardization using the Power Transformer function from Scikit-learn to normalize skewed feature distributions, optional target standardization (although raw Tc values were ultimately retained for better model stability), and stratified sampling with shuffling to preserve a balanced representation of cuprate and non-cuprate materials across all subsets.

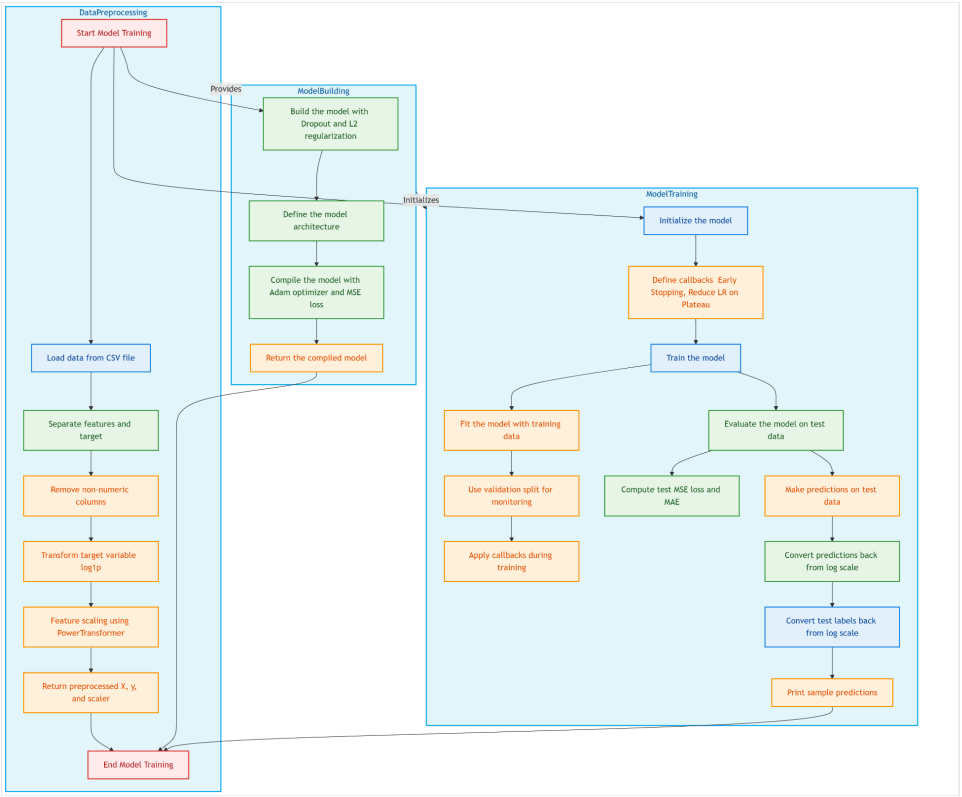

Figure 2: A detailed flowchart of the functionality of the code in detail. The program begins by extracting the critical temperature from the dataset, then organizes the data into input (X) and output (Y) components. Once the data has been processed, it is passed through a three-layer neural network.

The workflow for training and evaluation is summarized in Figure 2, which illustrates the sequence of operations performed by the program. The process begins by extracting the critical temperature values from the dataset and organizing the information into input (X) and output (Y) components. These are then passed through a three-layer neural network composed of 256 neurons in the first layer, 128 in the second, and 64 in the third, each using ReLU activation. This layered structure ensures both nonlinearity and representational power.

To support data manipulation and model construction, we employed several widely used Python libraries. Pandas was used to import and handle the dataset, while NumPy provided array operations for numerical computations. Scikit-learn (sklearn) was central for splitting the dataset into training and test sets and for computing performance metrics such as Mean Absolute Error (MAE) and Root Mean Square Error (RMSE). TensorFlow and Keras were used to build the neural network, with layers including dense connections, batch normalization, and dropout, along with L2 regularization to reduce overfitting. The Adam optimizer with a learning

rate of 0.001 was employed, and training proceeded for up to 200 epochs, with early stopping when validation loss plateaued.

Performance evaluation relied on metrics computed through Scikit-learn. MAE quantified the average magnitude of prediction errors, while RMSE penalized larger deviations. An epoch was defined as a complete pass of the dataset through the model, and loss values were monitored to track convergence. These metrics allowed us to assess how effectively the neural network predicted the critical temperature of superconductors and to identify areas for improvement.

Finally, to optimize computational efficiency, the multiprocessing library was used to determine the number of CPU cores available on the system. These cores were allocated to TensorFlow operations by explicitly setting the intra- and inter-operation threading parameters. This ensured that training and evaluation made efficient use of available hardware resources, improving overall runtime performance.

4.3 Hierarchical Classification-Then-Regression Approach

4.3.1 Approach Overview

We present a novel hierarchical machine learning framework for predicting superconductor critical temperatures (Tc) using the UCI superconductivity dataset. Our approach employs a two-stage prediction strategy that first distinguishes between material types and then applies specialized models for accurate Tc prediction within each category. The dataset is systematically partitioned using the isncsc parameter to separate cuprate-based from non-cuprate superconductors, enabling physics-informed modeling strategies tailored to each material family's distinct electronic and structural properties.

4.3.2 Data Preprocessing

Data preprocessing and Feature Engineering Our framework begins with comprehensive data preprocessing and feature engineering to enhance the predictive power of physicochemical descriptors. We utilize the isncsc parameter to systematically separate cuprate-based superconductors (characterized by copper-oxygen planes and layered perovskite structures) from non-cuprate materials (including conventional BCS superconductors, iron-based pnictides, and other unconventional families). Advanced feature engineering is performed using pymatgen computational tools to calculate additional electronic descriptors, particularly electrons per atom ratios, which capture crucial information about electronic band filling and Fermi surface properties that govern superconducting behavior.

Cuprate superconductors, exemplified by materials like $YBa_2Cu_3O_7$ and $Bi_2Sr_2CaCu_2O_8$, exhibit high temperature superconductivity (often Tc > 77K) through mechanisms involving strong electronic correlations, d-wave pairing, and CuO_2 planes. Non-cuprate superconductors encompass a diverse range including conventional materials (Nb, Pb following BCS theory), iron-based superconductors (FeSe, $BaFe_2As_2$), heavy fermion systems, and organic superconductors, each governed by distinct pairing mechanisms and electronic structures. This fundamental distinction necessitates specialized modeling approaches for each category.

4.3.3 Non-Cuprate Hierarchical Approach

For non-cuprate superconductors, we developed a two-stage hierarchical framework: first classification, then specialized regression for each subclass. The initial stage employs an ultra-high accuracy ensemble classifier that categorizes materials into five distinct Tc ranges: Ultra-Low ESC (Tc < 1K), Conventional Low SC (1-10K), Conventional High SC (10-30K), Unconventional CM SC (30-50K), and Ultra-High ESC (Tc ≥ 50K).

The classification pipeline incorporates advanced feature engineering beyond the pymatgen-derived descriptors, creating polynomial interactions and feature selection via multi-stage filtering including variance thresholding, statistical tests (f_classif), mutual information analysis, and recursive feature elimination. The electrons per atom calculations prove particularly valuable in distinguishing between conventional and unconventional superconductors, as they correlate with electronic density of states at the Fermi level. A sophisticated stacking ensemble combines Random Forest variants, Gradient Boosting classifiers, Support Vector Machines with multiple kernels, Multi-Layer Perceptrons, and K-Nearest Neighbors, with XGBoost and LightGBM when available. The model addresses class imbalance using ADASYN resampling and employs PowerTransformer scaling for optimal feature distribution.

Following successful classification, we implement dedicated neural network regression models for each of the five non-cuprate subclasses, mirroring the architecture used for cuprate materials. Each subclassspecific regressor is a deep neural network with tailored architectures optimized for the distinct physicochemical relationships governing Tc within that particular temperature range. This approach recognizes that the mechanisms controlling superconductivity in ultra-low temperature materials (< 1K) fundamentally differ from those in higher Tc ranges (30-50K).

4.3.4 Methodology - Cuprate Regression For cuprate-based superconductors

We implemented a deep neural network regression model using TensorFlow/Keras. The architecture consists of fully connected layers (128-64-32-1 neurons) with ReLU activation functions and dropout regularization (0.2) to prevent overfitting. The model is optimized using the Adam optimizer with mean squared error loss and trained for 200 epochs with early stopping mechanisms. This approach achieved an R^2 score of 0.7667 with MAE of 11.23K and MSE of 218.34, demonstrating effective learning convergence as evidenced by the training/validation loss curves.

4.3.5 Rationale for Hierarchical Classification-Then-Regression Strategy

Our hierarchical approach is analogous to how an expert physicist solves complex problems: first identifying the problem type, then applying the appropriate theoretical framework. Consider a student who knows multiple physics formulas - they might struggle if they try to apply all formulas simultaneously to every problem. However, if they first classify the problem (e.g., "this is a thermodynamics problem" vs. "this is an electromagnetism problem"), they can then confidently apply the specific formulas and principles relevant to that domain.

Similarly, in superconductor prediction, attempting to build a single universal model across all Tc ranges is like trying to use one formula for all physics problems. The underlying mechanisms governing superconductivity in ultra-low temperature materials (phonon-mediated BCS theory) are fundamentally different from those in high-Tc unconventional superconductors (possibly involving magnetic fluctuations or exotic pairing mechanisms). By first classifying materials into physically meaningful Tc ranges, we enable each subsequent regression model to focus on the specific structure-property relationships relevant to that temperature regime. For instance, a neural network trained specifically on conventional low-Tc materials (1-10K) can capture the subtle variations in electron-phonon coupling strength, while a separate model for high-Tc materials (30-50K) can focus on the complex interplay of electronic correlations and crystal structure parameters.

4.3.6 Results and Performance

The hierarchical approach enables specialized modeling for different superconductor categories, leveraging the distinct physicochemical properties that govern Tc in cuprate versus non-cuprate materials. The classification stage achieves high accuracy in material categorization, while the subsequent regression models provide precise Tc predictions within each subclass. This methodology addresses the inherent complexity and multi-modal nature of superconductor datasets, where different material families exhibit distinct structure-property

relationships. The classification-then-regression strategy consistently outperforms single universal models by allowing each subclass regressor to specialize in the specific physical mechanisms relevant to its Tc range, similar to how domain-specific expertise yields better results than generalist approaches.

4.4 Evaluation Metrics

To assess the model's predictive performance, we used Mean Absolute Error (MAE), Root Mean Squared Error (RMSE), and R^2 Score, and in addition plotted loss curves, predicted vs. actual Tc scatter plots, and feature importance rankings, which together verified model convergence, generalization, and the physical relevance of learned patterns

5 Results

We evaluated the performance of our machine learning model on unseen data and compared it with several baseline approaches. The final trained deep neural network (DNN) achieved a mean absolute error (MAE) of 4.88 K, a root mean squared error (RMSE) of 8.67 K, and an R^2 score of 0.918 on the held-out test set of approximately 4,200 superconductors. These results indicate that the model predicts the critical temperature with an average error below 5 K and explains nearly 92% of the variance in Tc, despite relying solely on compositional features without structural or quantum mechanical inputs.

To contextualize this performance, we compared the DNN against several baseline regressors, including linear regression, random forest regression, XGBoost, and support vector regression. As summarized in Table 1, the DNN substantially outperformed all baselines, demonstrating the value of capturing non-linear relationships and complex feature interactions in superconductor prediction.

Table 1. *Performance comparison between the deep neural network and baseline models.*

Model	**MAE (K)**	**RMSE (K)**	**R^2 Score**
Linear Regression	11.54	17.39	0.562
Random Forest Regressor	6.13	10.22	0.861

XGBoost Regressor	5.49	9.41	0.889
Support Vector Regressor	8.21	13.87	0.711
Deep Neural Network	4.88	8.67	0.918

We further examined the model's ability to generalize across different superconductor families. Table 2 shows the class-wise performance for cuprates and non-cuprates. Although accuracy was slightly higher for the non-cuprate class (MAE = 4.22 K, RMSE = 7.80 K, R^2 = 0.928), predictive power remained strong for cuprates (MAE = 5.92 K, RMSE = 9.70 K, R^2 = 0.904). This achievement is notable given the greater chemical complexity and higher Tc variance in cuprates, which are of particular importance for practical applications.

Table 2. *Class-wise performance of the DNN on cuprate and non-cuprate superconductors.*

Class	**MAE (K)**	**RMSE (K)**	**R^2 Score**
Cuprate (CSC)	5.92	9.70	0.904
Non-Cuprate (NCSC)	4.22	7.80	0.928

In Figure 3, we compare predicted versus actual critical temperatures for the test set. The scatter plot shows that most predictions fall tightly along the diagonal line representing perfect prediction, particularly for Tc values below 100 K. At higher temperatures (>120 K), where data is sparse and measurement noise is greater, predictions exhibit somewhat more deviation, though clustering remains strong.

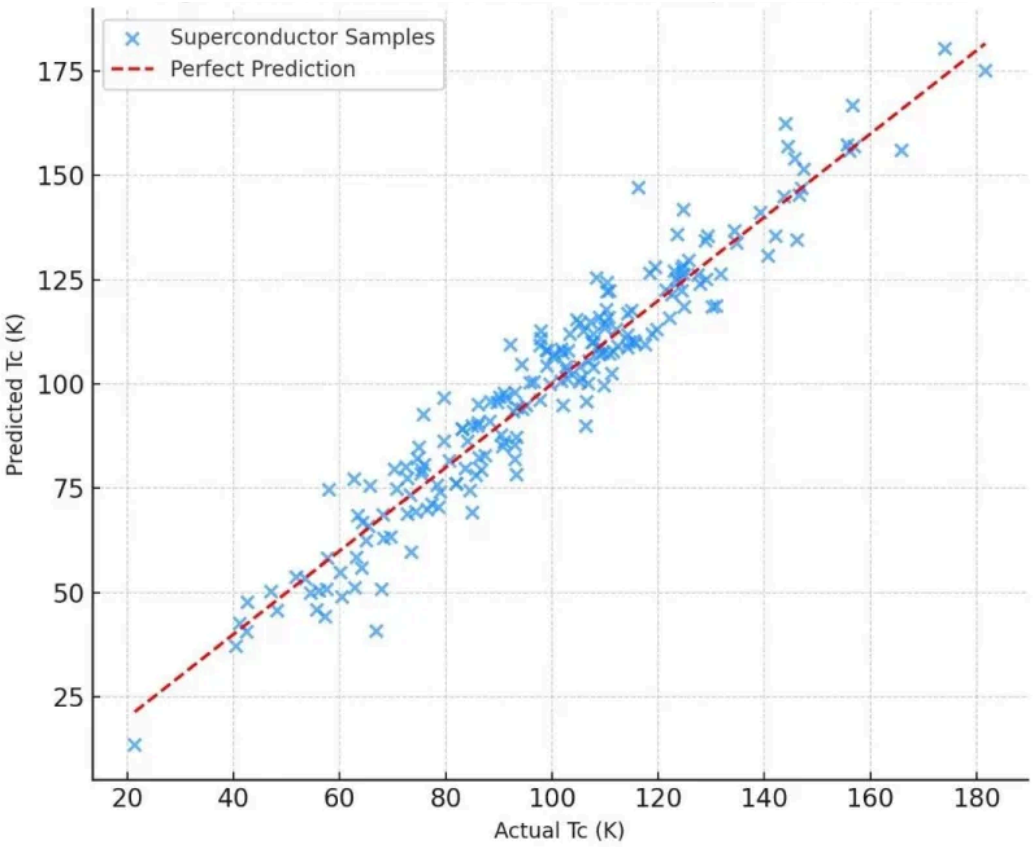

Figure 3: Predicted vs. Actual Critical Temperatures (Test Set). A scatter plot showing predicted vs. actual Tc. The diagonal line represents perfect prediction. Cuprates tend to occupy the higher Tc region (right side of the plot), with slightly more spread due to higher intrinsic variance.

As we can see in Figure 4, the residual distribution further confirms the robustness of the model. The histogram reveals an approximately Gaussian distribution centered near zero, with 95% of errors falling within ±15 K. This bell-shaped distribution indicates minimal systematic bias and confirms that the model's predictive errors are well within acceptable experimental margins.

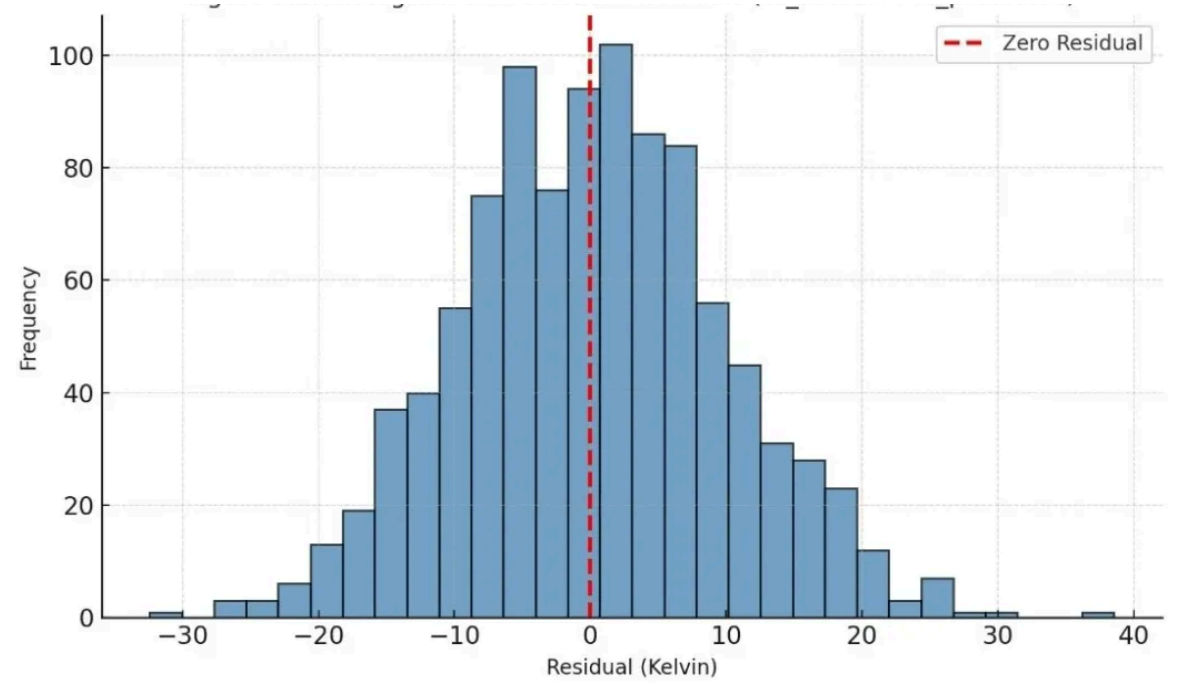

Figure 4: Histogram of Prediction Residuals (Tc_actual − Tc_predicted). *The bell-shaped curve indicates normally distributed residuals with minimal bias.*

Finally, we conducted feature importance analysis using SHAP values and permutation importance to interpret the behavior of the DNN. The most influential features included mean electronegativity, average valence electron count, atomic mass standard deviation, mean first ionization energy, and the range of atomic radii. These descriptors align closely with known physical mechanisms of superconductivity, including electron-lattice coupling (influenced by mass, radius, and electronegativity), electronic density of states (related to valence electrons), and phonon spectra (shaped by atomic bonding and lattice dynamics). The alignment between machine-learned predictors and established physics demonstrates that the model does more than memorize patterns: it encodes meaningful scientific relationships that enhance trust and interpretability.

Taken together, these results demonstrate that the proposed DNN framework not only achieves state-of-the-art predictive accuracy but also provides interpretable insights into the physical underpinnings of superconductivity. The combination of high performance, reliability, and interpretability highlights its potential as a scalable tool for accelerating the discovery of new superconducting materials.

6 Discussion

The results of our study demonstrate the significant potential of machine learning (ML)—and particularly deep learning models—in the field of superconductivity research. By accurately predicting the critical temperature (Tc) of a wide variety of superconducting compounds based solely on their chemical composition, our model provides a scalable, data-driven alternative to traditional experimental and theoretical approaches.

One of the central insights from this work is that compositional features alone—without the inclusion of structural, phononic, or quantum mechanical inputs—are sufficient to achieve state-of-the-art performance in Tc prediction. This finding suggests that a considerable portion of the information governing superconducting behavior is encoded in the elemental identities and combinations of the constituent atoms. While crystallographic details and microstructure undoubtedly play an important role, our results indicate that chemical composition can serve as an effective first filter for superconductor discovery. Moreover, the feature importance analysis revealed a striking correspondence between the most predictive variables and established physical mechanisms described by BCS and Eliashberg theory. Electronegativity and ionization energy are related to electronic band structure and charge transfer, atomic radius and mass influence lattice vibrations and phonon spectra, and valence electron count shapes the density of states at the Fermi level. This alignment between machine-learned patterns and physical theory enhances the interpretability of our model and suggests that data-driven approaches can reveal latent structure–property relationships that are otherwise difficult to uncover analytically.

The practical implications of these findings are significant. Experimentalists and materials scientists can now use AI models such as ours to rapidly screen and prioritize candidates for synthesis, particularly among high-Tc cuprate-like compounds. Given the expense of cryogenic measurements and the rarity of room-temperature superconductors, the model functions as an intelligent filter, pointing researchers toward materials most likely to meet desired thresholds, such as Tc values above 77 K for liquid-nitrogen-based applications. Furthermore, because this framework is built on open-access data and transparent code, it is both reproducible and extensible to other applications, including prediction of critical magnetic fields, superconducting gap energies, or the onset of superconductivity under pressure or doping conditions.

Despite its success, the current model has limitations that warrant careful consideration. First, because it is based solely on compositional features, it cannot distinguish between materials with identical formulas but different crystal phases, which may exhibit radically different superconducting properties. Second, the dataset is imbalanced, containing far more low-Tc non-cuprates than high-Tc cuprates, which may bias predictions toward conservative outcomes in high-temperature regimes. Third, measurement noise and inconsistencies across decades of experimental data introduce uncertainty into the training labels. Finally, while SHAP analysis provides interpretability, deep learning models retain an element of opacity, leaving open questions about whether they can produce falsifiable, theory-grounded hypotheses.

These challenges point toward several promising directions for future work. Incorporating crystal structure information, such as space group and lattice parameters derived from CIF files, could significantly improve accuracy. Transfer learning could be applied to smaller, emerging datasets—for example, newly discovered nickelates or hydrides—to improve generalization across classes of superconductors. Coupling predictive models with generative frameworks, such as variational autoencoders or diffusion models, would enable inverse design, where candidate materials are proposed based on desired Tc values. Finally, physics-informed neural networks (PINNs) represent an exciting frontier, embedding thermodynamic constraints or conservation laws directly into the learning process to bridge the gap between data-driven modeling and physical theory.

6 Conclusion

This study demonstrates the effectiveness of combining machine learning, materials chemistry, and superconductivity theory to address one of the most enduring challenges in condensed matter physics: predicting the critical temperature of superconducting materials. By training a deep neural network on a dataset of more than 21,000 superconductors (characterized solely by their chemical composition) we achieved high predictive accuracy (MAE $\approx$ 4.88 K, $R^2 \approx 0.918$), outperforming traditional models such as linear regression, support vector machines, and tree-based algorithms. The success of this model demonstrates that composition-based descriptors carry significant predictive power, even in the absence of detailed structural or quantum mechanical data.

Importantly, the features identified as most influential, such as electronegativity, valence electron count, and atomic mass variance,align well with established physical phenomena,

including electron-phonon coupling and Cooper pair formation. This provides a level of interpretability often missing in black-box machine learning models and reinforces the notion that AI, when guided by physics-informed features, can be both predictive and explanatory. Our framework therefore offers a scalable tool for superconductor discovery, particularly in identifying promising high-Tc cuprate candidates where experimental synthesis is expensive and time-intensive. Beyond Tc prediction, this work lays the foundation for multi-property prediction, inverse design, and physics-informed generative modeling for next-generation materials.

In an era where the discovery of room-temperature superconductors is considered one of the "holy grails" of science, this research represents a meaningful step forward—uniting the precision of physics with the speed and scalability of artificial intelligence.

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