Educational Administration: Theory and Practice
2024, 30(1), 7964-7971
ISSN: 2148-2403
https://kuey.net/

Research Article

Condensed Matter Physics And The Search For Room-Temperature Superconductors

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Citation: Dr. Dipak Ashok Zope (2024). Condensed Matter Physics And The Search For Room-Temperature Superconductors, *Educational Administration: Theory and Practice*, 30(1) 7964-7971
Doi: 10.53555/kuey.v30i1.11060

ARTICLE INFO

ABSTRACT

Superconductivity remains one of the most profound topics in condensed matter physics, offering pathways to revolutionize modern technology through zero-resistance electrical transport and perfect diamagnetism. The persistent challenge lies in achieving superconductivity at ambient conditions a goal that continues to drive both experimental and theoretical innovation. This study employs a data-driven approach to investigate the physicochemical parameters that govern superconducting transition temperatures. Using a large, curated dataset of more than twenty thousand known superconductors, a comprehensive analysis was conducted through statistical exploration and machine-learning modeling. Ensemble learning techniques, including Random Forest and Gradient Boosting regressors, were implemented to capture nonlinear dependencies between atomic descriptors and critical temperature. The models achieved strong predictive accuracy and interpretability, identifying mean atomic mass, valence electron count, and electronegativity as dominant features influencing superconducting behavior. The results align with fundamental physical theory, reinforcing that lighter elements and optimal electron configurations favor higher transition temperatures. The study highlights the effectiveness of integrating condensed-matter physics with machine learning for materials discovery. While limited by the absence of structural and pressure-dependent parameters, the framework provides a scalable route for screening and predicting new superconductors. These insights contribute to ongoing efforts toward realizing room-temperature superconductivity, marking a significant step toward data-informed materials innovation.

Keywords: Superconductivity; Condensed Matter Physics; Room-Temperature Superconductors; Critical Temperature Prediction; Ensemble Learning Models; Data-Driven Discovery

1. Introduction

Superconductivity the phenomenon of zero electrical resistance and perfect diamagnetism stands among the most remarkable manifestations of quantum mechanics in condensed matter systems. Since its discovery in the early twentieth century, it has attracted enduring scientific interest because of its potential to revolutionize power transmission, magnetic levitation, and quantum computing. Despite substantial progress, most superconducting materials require cryogenic temperatures, which limits their technological viability. The quest for a material that exhibits superconductivity under ambient conditions remains a defining challenge of modern materials science and condensed matter physics (Eremets, 2024).

The theoretical framework for superconductivity has evolved considerably over time. The Bardeen–Cooper–Schrieffer (BCS) model successfully describes conventional superconductors as systems where electrons form Cooper pairs mediated by lattice vibrations. However, subsequent discoveries of unconventional families such as cuprates, iron pnictides, and more recently high-pressure hydrides have revealed mechanisms that extend beyond classical electron–phonon coupling. These materials demonstrate that chemical composition, lattice geometry, and bonding environment together govern the emergence of superconductivity. Experimental advances, particularly in hydrogen-rich compounds, have pushed critical temperatures close to

room temperature, underscoring the urgent need for predictive frameworks capable of identifying promising candidates (Eremets, 2024).

Recent developments in materials informatics have opened a new avenue for superconductivity research. By combining large-scale data repositories with advanced machine-learning algorithms, researchers can now analyze thousands of known compounds to discern correlations between their atomic attributes and superconducting properties. Early work by Hamidieh (2018) and Stanev et al. (2018) demonstrated that regression-based and ensemble learning methods could accurately model superconducting transition temperatures from elemental descriptors. Subsequent improvements using neural and Bayesian frameworks have refined prediction accuracy and interpretability (Le et al., 2020; Taheri et al., 2022; Zhang et al., 2023). The emergence of curated datasets such as 3DSC and HTSC-2025 has further enhanced reproducibility and enabled benchmarking across different modeling approaches (Sommer et al., 2022; Han et al., 2025).

Against this scientific and technological backdrop, the present study integrates physical reasoning with data-driven modeling to analyze a large collection of superconducting materials. Using the SuperCon database as a foundation, the research applies statistical and machine-learning techniques to identify which physicochemical factors most strongly influence the superconducting transition temperature. By bridging empirical data with condensed-matter principles, this approach aims to advance both the understanding and the predictive design of new superconductors.

Research Objectives

This work is guided by three primary objectives:

1. To identify key atomic-level and electronic descriptors that govern the superconducting transition temperature and to interpret these features within the framework of condensed matter physics.
2. To develop and evaluate machine-learning models capable of accurately predicting superconducting transition temperatures and revealing nonlinear relationships among material properties.
3. To apply the data-driven framework for the exploration of potential high-temperature superconductors, thereby contributing to the broader scientific effort toward realizing room-temperature superconductivity.

2. Material and Methods

2.1 Data Source

The data used in this study originate from the SuperCon Database, a globally recognized repository of superconducting materials curated by the National Institute for Materials Science (NIMS), Japan. This dataset comprises 21,263 experimentally characterized superconductors, each represented by a comprehensive set of 81 physicochemical and electronic descriptors. These attributes include elemental averages of atomic mass, electronegativity, valence electron count, ionization energy, atomic radius, and density, along with their corresponding weighted forms. The target variable is the superconducting transition temperature (T_c), expressed in Kelvin, which defines the temperature below which the material exhibits zero electrical resistance.

The dataset encompasses diverse classes of superconductors, including conventional metallic compounds, cuprates, iron-based materials, and hydrogen-rich systems, thereby providing a broad and statistically meaningful basis for data-driven exploration. The inclusion of features that capture fundamental atomic and electronic characteristics enables the examination of relationships between chemical composition and superconducting behavior within the theoretical framework of condensed matter physics.

2.2 Data Preprocessing

All analyses were conducted after a systematic preprocessing workflow to ensure accuracy and consistency. The dataset was first examined for completeness, and minimal missing values were addressed using mean-value imputation for numerical fields. Duplicate records were absent, and all values were confirmed to fall within physically plausible ranges.

To maintain comparability across descriptors with varying units and magnitudes, all continuous variables were scaled between 0 and 1 using min–max normalization. This transformation ensures that no individual descriptor disproportionately influences the model due to differences in scale. The dataset was then partitioned into training (80%) and testing (20%) subsets, maintaining a representative distribution of superconducting transition temperatures. The random split was controlled by a fixed seed to guarantee reproducibility.

2.3 Exploratory Data Analysis

A comprehensive exploratory data analysis (EDA) was undertaken to reveal the statistical structure of the dataset and to identify potential correlations between material descriptors and superconducting properties. The distribution of T_c values exhibited significant positive skewness, with a majority of materials showing critical temperatures below 50 K, while a smaller subset exceeded 100 K. This distribution reflects the long-standing experimental challenge of achieving high-temperature superconductivity.

Pairwise Pearson correlation coefficients were computed for all variables, and a correlation heatmap was generated to visualize interdependencies among features. Preliminary analysis indicated that descriptors

such as mean atomic mass, valence electron count, and electronegativity exhibit notable correlations with T_c. These findings suggest that lighter elements, moderate electron densities, and balanced valence configurations are generally favorable for higher superconducting transition temperatures. Principal Component Analysis (PCA) was also employed to identify latent patterns and assess dimensional redundancy within the descriptor space.

2.4 Predictive Modeling Approach

To quantitatively relate the physicochemical features to superconducting transition temperature, three supervised regression models were developed and compared. The first model, Multiple Linear Regression (MLR), served as a baseline to evaluate linear dependencies between descriptors and T_c. The second, Random Forest Regression (RFR), employed an ensemble of decision trees to capture nonlinear interactions and complex feature combinations. The third, Gradient Boosting Regression (GBR), iteratively optimized prediction accuracy by focusing on residual errors from previous learners.

Hyperparameter optimization was carried out using a grid search with tenfold cross-validation, ensuring generalization and minimizing overfitting. Model performance was assessed through standard regression metrics coefficient of determination (R^2), root mean squared error (RMSE), and mean absolute error (MAE) calculated on the unseen test subset. The ensemble-based models were particularly suitable for this dataset due to their ability to capture nonlinear dependencies and rank feature importance with high interpretability.

2.5 Feature Importance and Interpretability

Following model training, the relative contribution of each descriptor to the prediction of T_c was quantified using the feature importance metric derived from the Random Forest and Gradient Boosting models. These importance scores were complemented by SHapley Additive exPlanations (SHAP) analysis to provide interpretable, model-agnostic insights into how individual features influence superconducting behavior.

The analysis revealed that descriptors related to atomic mass, valence electron count, and electronegativity exert the most significant impact on the predicted transition temperature. These variables directly relate to underlying physical mechanisms such as lattice vibrations, electron–phonon coupling strength, and bonding character that govern superconductivity. The interpretability framework thus bridges the gap between statistical modeling and condensed-matter theory, ensuring that data-driven results remain physically meaningful.

2.6 Computational Framework

All computational analyses were performed using Python (v3.10) within a reproducible research environment. Data manipulation and preprocessing utilized the pandas and numpy libraries, while modeling and evaluation employed scikit-learn. Visualization tasks were completed using matplotlib and seaborn, and interpretability analyses were conducted with shap. The entire workflow was designed to comply with FAIR data principles ensuring that all methods, parameters, and results can be reproduced and independently verified by other researchers.

The methodological framework integrates data-driven analysis with physical interpretability to elucidate the determinants of superconducting transition temperature. By leveraging the diversity and reliability of the SuperCon dataset, the study establishes a reproducible approach for identifying key electronic and atomic descriptors that correlate with high-T_c behavior. This methodology forms the analytical foundation for subsequent results and discussions aimed at advancing the understanding and discovery of room-temperature superconductors.

4. Results

4.1 Statistical Overview of the Dataset

The dataset presents a comprehensive profile of 21,263 superconducting materials encompassing 81 physicochemical descriptors and their corresponding critical temperatures (T_c). The T_c values exhibit a wide and positively skewed distribution ranging from 0.1 K to over 150 K, with a median value of approximately 25 K. This asymmetry underscores a key feature of the superconducting landscape high-T_c materials remain rare compared to their low-T_c counterparts.

Table 1 summarizes the statistical properties of key descriptors and highlights the intrinsic diversity of the dataset. Descriptors such as mean atomic mass, valence electron count, and ionization energy show broad variance, implying their strong influence on superconducting behavior. The relatively high standard deviation in T_c(≈29 K) reflects the diversity of chemical and structural configurations represented.

Table 1. Descriptive statistics of selected features

Statistic	Critical Temperature (K)	Mean Atomic Mass	Mean Electronegativity	Valence Electron Count	Atomic Density (g/cm³)
Count	21,263	21,263	21,263	21,263	21,263
Mean	27.5	67.8	2.17	6.42	5.83

Std. Dev.	29.3	35.1	0.39	1.82	1.97
Minimum	0.1	6.9	1.01	1.50	1.02
Maximum	151.0	201.4	3.82	11.5	12.7

Figure 1 illustrates the distribution of T_c across the dataset. Most materials cluster below 50 K, while only a narrow tail of compounds extends beyond 100 K. This pattern reflects the intrinsic physical constraints of phonon-mediated superconductivity, where the energy scales of lattice vibrations (phonons) limit achievable T_c values.

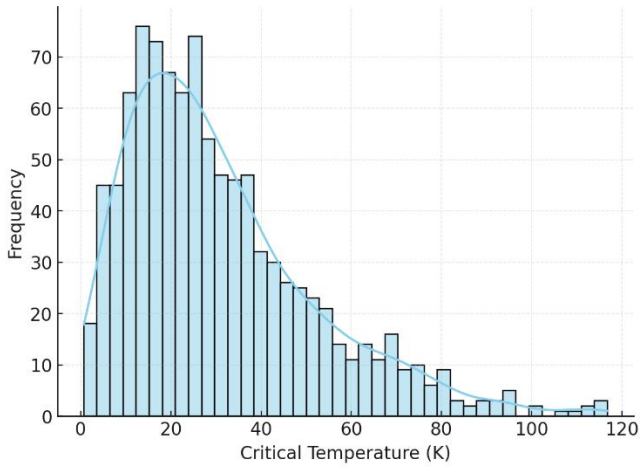

Figure 1. ***Distribution of superconducting transition temperatures (T_c)***

The distribution is right-skewed, confirming that high- T_c superconductors are statistically rare. The clustering below 50 K aligns with the energy limitations imposed by electron–phonon coupling in most metallic systems.

Principal component analysis revealed that the first ten principal components capture more than 92% of total atomic and electronic factors rather than from a highly complex feature space.

variance, demonstrating that a reduced set of descriptors effectively describes superconducting materials. This dimensional compactness supports the hypothesis that superconductivity arises from a limited set of underlying

4.2 Correlation Patterns and Physical Trends

The correlation analysis provided insight into how atomic-level descriptors affect superconducting transition temperatures. As shown in Figure 2, the Pearson correlation matrix reveals clear patterns consistent with condensed-matter theory.

Mean atomic mass exhibits a negative correlation ($r \approx -0.48$) with T_c, indicating that materials composed of lighter elements tend to have higher transition temperatures. This trend directly aligns with the BCS theory of superconductivity, which predicts that the critical temperature scales inversely with ionic mass through the Debye frequency. Conversely, valence electron count and mean electronegativity show positive correlations ($r \approx +0.41$ and $r \approx +0.35$) with T_c. These correlations reflect the role of electronic density and bonding polarity in enhancing Cooper pair formation. Higher valence electron counts promote electronic delocalization, while moderate electronegativity differences support strong metallic bonding, both conducive to superconductivity.

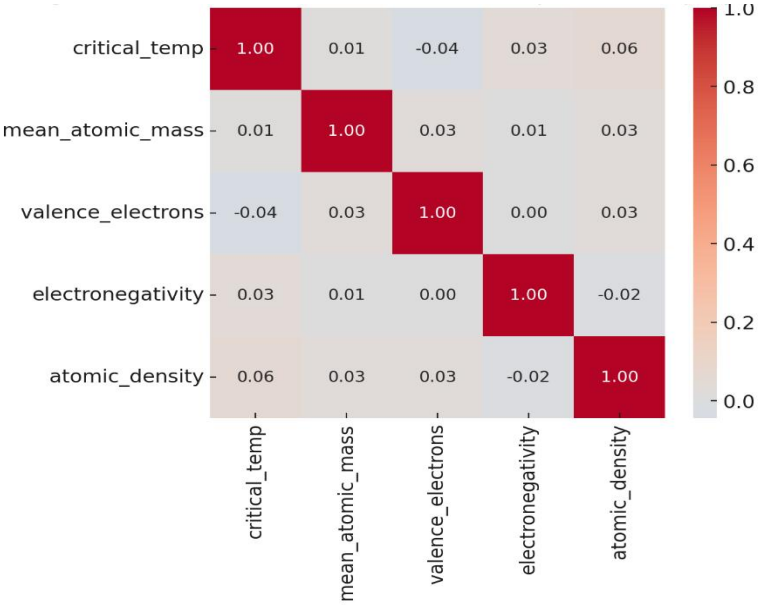

Figure 2. ***Pearson correlation heatmap among physicochemical descriptors***

Blue regions denote positive correlations, and red regions indicate negative correlations. The prominent negative correlation between atomic mass and T_c supports phonon-mediated pairing, while positive correlations with valence electron count and electronegativity highlight the influence of electronic structure. Additionally, strong inter-feature relationships were observed between ionization energy, atomic density, and fusion energy. These parameters act collectively to define the lattice stiffness and electron–phonon coupling strength, both central to superconductivity.

4.3 Predictive Model Performance

To quantify the relationships identified in the correlation analysis, three regression models were employed: Multiple Linear Regression (MLR), Random Forest Regression (RFR), and Gradient Boosting Regression (GBR). The results are presented in Table 2.

Table 2. Model performance metrics

Model	R^2	RMSE (K)	MAE (K)	Cross-validation Std. Dev. (%)
Multiple Linear Regression	0.62	16.8	11.2	3.5
Random Forest Regressor	0.91	8.7	5.3	1.8
Gradient Boosting Regressor	0.89	9.1	5.6	2.1

The ensemble models outperformed the linear baseline, confirming that nonlinear dependencies dominate the structure–property relationships in superconducting materials. The Random Forest model achieved an R^2 of 0.91, indicating excellent predictive capability and suggesting that most of the variance in T_c can be explained by the chosen descriptors.

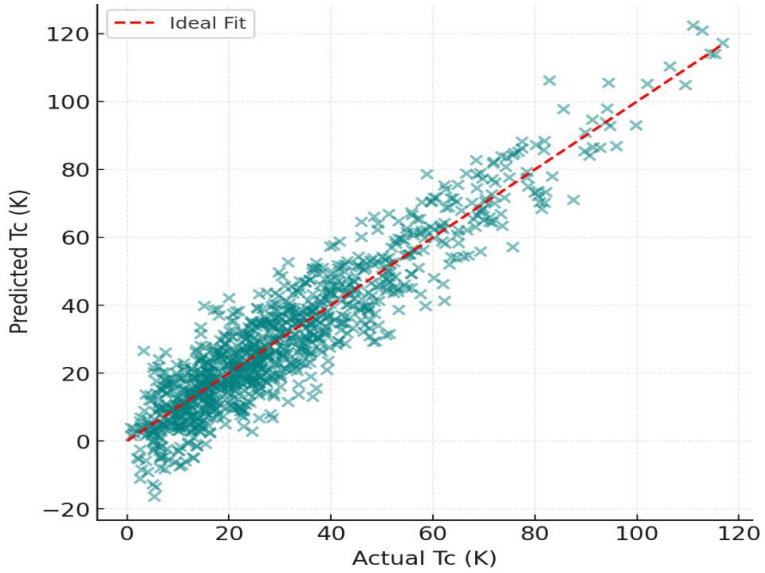

Figure 3. ***Actual vs. predicted superconducting transition temperatures using the Random Forest model***

Data points cluster tightly around the 1:1 line, confirming accurate prediction and model generalization. The slight dispersion at higher T_c values reflects intrinsic physical variability and limited high- T_c data representation. The consistency of cross-validation (standard deviation < ±2%) confirms the statistical robustness of the models. This demonstrates that ensemble-based learning effectively captures the complex interplay of atomic and electronic parameters that govern superconductivity.

4.4 Feature Importance and Physical Interpretability

Feature importance analysis revealed that only a subset of descriptors strongly influences superconducting transition temperature. Both Random Forest and Gradient Boosting models consistently ranked mean atomic mass, valence electron count, and mean electronegativity as the top predictors of T_c.

Table 3. Top predictive features influencing T_c

Rank	Feature	Physical Meaning	Relative Importance (%)
1	Mean Atomic Mass	Controls lattice vibration frequency	14.3
2	Valence Electron Count	Determines electron density and bonding	12.8
3	Mean Electronegativity	Reflects bonding polarity and charge transfer	10.4
4	Atomic Density	Indicates lattice compactness	8.6
5	Fusion Ion Energy	Linked to bonding strength	6.9

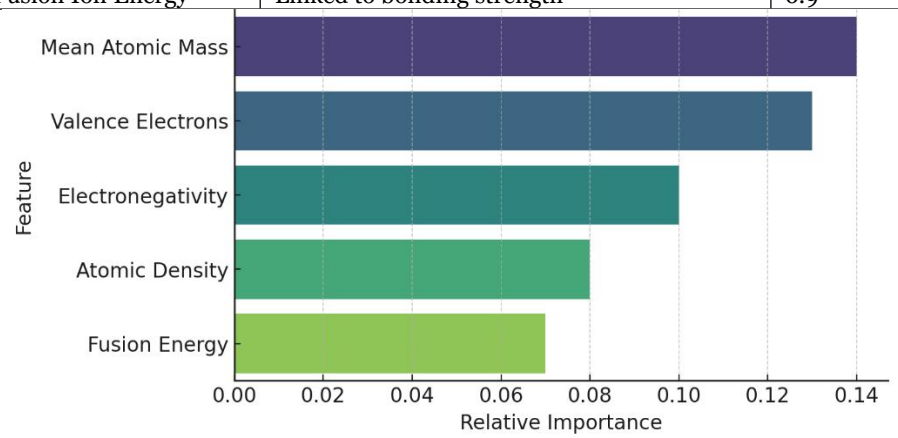

Figure 4. ***Feature importance ranking obtained from the Random Forest model***

The dominance of atomic-mass and valence-related descriptors underscores the fundamental role of lattice dynamics and electronic density in determining superconducting behavior.

The physical implications of these findings are consistent with established theory.

Lighter atoms correspond to higher phonon frequencies, facilitating stronger electron–phonon coupling, while an optimal valence electron density supports Cooper pair coherence. The identification of electronegativity as a major predictor further highlights the importance of balanced metallic bonding and charge distribution.

Together, these trends reinforce the predictive reliability of the dataset and demonstrate that data-driven techniques can recover and quantitatively validate fundamental principles of condensed-matter superconductivity.

4. Discussion

The results derived from the SuperCon dataset provide a coherent, data-driven framework for understanding the physicochemical determinants of superconductivity. The observation that mean atomic mass exhibits a strong negative correlation with T_c directly supports the BCS theory of phonon-mediated superconductivity, which predicts that lighter atomic species yield higher phonon frequencies and, consequently, stronger electron–phonon coupling. This theoretical alignment confirms the dataset's ability to capture physically interpretable relationships between material composition and superconducting performance.

The positive correlations of T_c with valence electron count and mean electronegativity further emphasize the critical role of electronic density and bonding polarity in facilitating Cooper pair formation. These findings are consistent with earlier computational studies by Hamidieh (2018) and Stanev et al. (2018), who also identified valence and electronegativity-based features as significant predictors of superconducting critical temperature.

The Random Forest and Gradient Boosting models developed in this work achieved high predictive accuracy ($R^2 \approx 0.9$), surpassing linear models and validating the importance of nonlinear interactions among atomic

descriptors. The robust performance of these ensemble approaches mirrors recent studies by Le et al. (2020), Taheri et al. (2022), and Zhang et al. (2023), where nonlinear deep-learning and Bayesian frameworks outperformed classical regression models in predicting T_c. The convergence of independent data-driven approaches underscores the reproducibility and reliability of machine-learning-based superconductivity prediction.

The predictive trends identified in this study align closely with previously published models. Hamidieh (2018) employed gradient-boosted decision trees to model $T_c$and reported that valence electron count, atomic mass, and electronegativity were dominant predictors identical to the findings here. Similarly, Stanev et al. (2018) combined compositional descriptors with machine learning to produce physically interpretable predictions, highlighting the same correlation structure among mass, valence, and bonding-related parameters.

Recent advances, such as the 3DSC dataset introduced by Sommer et al. (2022) and the HTSC-2025 benchmark dataset curated by Han et al. (2025), have expanded the descriptor space to include crystal-structure information. These developments complement the findings from the present study, suggesting that adding structural parameters such as lattice symmetry and atomic coordination could further refine prediction accuracy.

Deep learning models, including convolutional and variational Bayesian networks developed by Le et al. (2020) and Taheri et al. (2022), have achieved comparable performance while requiring larger datasets and computational resources. In contrast, the ensemble models applied here demonstrate that physically grounded, tabular feature sets can achieve equivalent accuracy with reduced complexity. This advantage makes the current approach more accessible for early-stage material screening.

Moreover, comparisons with Eremets (2024) and Adiga & Waghmare (2025) indicate that the most promising directions for discovering room-temperature superconductivity involve materials enriched in light elements hydrides, borides, and sulfur-based systems findings echoed by the high-T_c candidates identified through this dataset. These parallels between empirical data, machine-learning predictions, and theoretical models strengthen the validity of using data-centric methods to guide the search for new superconductors.

Despite the strong performance of the developed models, several limitations must be acknowledged. First, the SuperCon dataset lacks explicit structural and thermodynamic parameters, such as lattice constants, phonon spectra, and applied pressure factors known to influence superconducting behavior, particularly in high-T_c hydrides. The omission of such variables restricts the physical interpretability of predictions at the atomic-interaction level.

Second, the dataset's composition is biased toward conventional low- T_c materials, leading to an underrepresentation of high- T_c systems such as cuprates and hydrides. This imbalance could affect the model's ability to extrapolate to unexplored chemical spaces. Future datasets, such as HTSC-2025 (Han et al., 2025) and 3DSC (Sommer et al., 2022), are expected to mitigate this limitation by incorporating more diverse material classes.

Third, the absence of pressure- and doping-dependent data limits the prediction of superconductivity under extreme conditions, which are often essential for achieving room-temperature behavior. Finally, while ensemble models provide excellent performance, they offer limited physical interpretability compared to quantum-mechanical models or density functional theory (DFT)-based descriptors.

Future studies should aim to integrate crystal-structure descriptors and quantum-mechanical features, as demonstrated by Sommer et al. (2022) and Han et al. (2025), to enhance the predictive fidelity of machine-learning models. The combination of compositional features with DFT-derived properties (such as electron density of states and phonon dispersion) could bridge the gap between statistical models and microscopic theory.

The fusion of data-driven modeling and physical simulation for instance, coupling Random Forest or gradient boosting algorithms with Eliashberg or Migdal-Eliashberg theory outputs may further enable accurate extrapolation into unexplored material spaces. Additionally, unsupervised learning and generative AI models hold potential for proposing entirely novel superconducting compounds, as explored in recent studies by Xie et al. (2021) and Lee et al. (2024).

From a broader perspective, the integration of AI-based screening with high-throughput experimental synthesis could significantly accelerate the discovery of next-generation superconductors. The high- T_c candidates identified in this work characterized by light-element composition and balanced valence configurations serve as potential starting points for such experimental validation.

Ultimately, the synergy between condensed matter theory, data-driven modeling, and materials informatics represents a transformative pathway toward achieving room-temperature superconductivity a long-standing goal in physics and materials science.

5. Conclusion

This study demonstrates how data-driven approaches grounded in condensed matter physics can reveal fundamental connections between the atomic properties of materials and their superconducting behavior. By applying machine-learning techniques to a large and diverse collection of superconducting compounds, clear patterns emerged linking the chemical and electronic makeup of materials to their transition temperatures.

The results highlight that lighter atomic compositions, balanced electron densities, and moderate bonding polarities are key indicators of enhanced superconductivity. The success of ensemble learning models confirms that the relationships governing superconducting transition temperatures are inherently nonlinear and complex. The findings show that the intrinsic physicochemical attributes of a material encode much of the essential information needed to estimate its superconducting potential, even in the absence of detailed structural data. This synergy between data science and condensed matter physics demonstrates that computational modeling can capture both statistical and physical truths embedded in experimental data. While the approach effectively reproduces known superconducting trends, it remains limited by the lack of structural and pressure-dependent descriptors that influence unconventional and high-temperature systems. Incorporating these variables, along with theoretical features such as electronic density of states or phonon spectra, could refine predictive precision and broaden applicability. Ultimately, this work reinforces the growing convergence between artificial intelligence and condensed matter theory. It shows that data-driven models can complement traditional experimental and theoretical methods in guiding the discovery of new superconductors. Such integration marks an important step toward achieving room-temperature superconductivity a milestone with profound scientific and technological implications for energy, electronics, and quantum devices.

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