Machine-Learning-Guided Prediction Models of Critical Temperature of Cuprates

Dongeon Lee, Daegun You, Dongwoo Lee, Xin Li, and Sooran Kim

ABSTRACT: Cuprates have been at the center of long debate regarding their superconducting mechanism; therefore, predicting the critical temperatures of cuprates remains elusive. Herein, using machine learning and first-principles calculations, we predict the maximum superconducting transition temperature \( T_{c,\text{max}} \) of hole-doped cuprates and suggest the functional form for \( T_{c,\text{max}} \) with the root-mean-square-error of 3.705 K and \( R^2 \) of 0.969. We have found that the Bader charge of apical oxygen, the bond strength between apical atoms, and the number of superconducting layers are essential to estimate \( T_{c,\text{max}} \). Furthermore, we predict the \( T_{c,\text{max}} \) of hypothetical cuprates generated by replacing apical cations with other elements. Among the hypothetical structures, the cuprates with Ga show the highest predicted \( T_{c,\text{max}} \) values, which are 71, 117, and 131 K for one, two, and three CuO\(_2\) layers, respectively. These findings suggest that machine learning could guide the design of new high-\( T_c \) superconductors in the future.

Understanding the material dependence of superconducting temperature \( (T_c) \) has been a long-standing subject of importance in the condensed matter physics community. However, this becomes especially challenging for high-\( T_c \) cuprates, as their underlying mechanism of superconductivity, despite intensive experimental and theoretical studies, remains elusive over 30 years since the discovery of La\(_2\)CuO\(_4\).\(^{1}\) All cuprate superconductors share the common characteristics of a two-dimensional CuO\(_2\) superconducting layer and strong electronic correlations, while their experimental maximum superconducting transition temperatures \( (T_{c,\text{max}}) \) vary by an order of magnitude from the La family to the Hg family. This suggests that out-of-CuO\(_2\)-plane effects should also be integrated into the superconducting mechanism. Furthermore, complex physical phenomena such as abnormal phonons, charge density wave, and pseudo gap state bring continuous interest and discussion to copper-based superconductors.\(^{2,\text{a}}\)

Several material-dependent parameters that have strong correlations with \( T_c \) of cuprates have been suggested. Experimentally, the \( T_c \) increases with the number of CuO\(_2\) layers up to three and decreases beyond four.\(^{3,\text{a}}\) The apical oxygen height \( (d_{\text{apical}}) \), the distance between the apical oxygen and in-plane copper, has been considered to have a positive correlation with \( T_{c,\text{max}} \).\(^{4}\) Computationally, the axial orbital energy, the range parameter of the intralayer hopping,\(^{5}\) the Madelung potential of the apical oxygen,\(^{6}\) and the charge-transfer energy between the in-plane Cu and oxygen,\(^{7}\) all have been shown to correlate with the material dependence of \( T_{c,\text{max}} \). Recently, Kim et al. suggested the bond strength between apical atoms and the Bader charge of apical oxygen, which are related to phonons of the apical oxygen and out-of-CuO\(_2\)-plane charge fluxes, as material-dependent parameters.\(^{8}\)

A generalized flux picture to further emphasize the importance of dynamic anharmonic coupling of phonons and fluxes was shown to predict a few important experimental phenomena in the pseudogap and strange metal phases of cuprates.\(^{9}\)

Even though previous works have reported these significant correlations between certain parameters and \( T_c \), which helped understand material dependence, they often lack a quantitative analysis and prediction of the material dependence of \( T_c \) for the existing or nonexistent structures. On the other hand, the data-driven machine learning (ML) technique has been developed to predict the properties of materials without demanding a preknown exact mechanism.\(^{10-12}\) Especially, to predict \( T_{c,\text{max}} \), several studies have been reported using various ML algorithms and features for BCS-type,\(^{13-15}\) Fe-based,\(^{16-18}\) Cu-based,\(^{19-21}\) and a broad class of superconductors.\(^{22,23,26-32}\)

Features based on the chemical composition of materials are commonly used for ML modeling because of their accessibility. For example, Stanev et al. reported a random forest (RF) model predicting \( T_c \) of materials, including low-\( T_c \), Cu-based, and Fe-based superconductors using chemical features.\(^{23}\)

Received: May 4, 2021
Accepted: June 16, 2021
Published: July 1, 2021
However, the physical interpretability of the chemical composition features to the output prediction is not always directly understandable, along with black-box algorithms of ML. Recently, Xie et al. suggested an ML model in a functional form with the electron–phonon coupling (λ), logarithmic average phonon frequency (ωlog), and Coulomb pseudopotential (μ*) for BCS-type superconductors. Along this line, it would be worth exploring the direct relationship between material-dependent parameters of cuprates and their Tc using ML. In this work, we aim to develop ML models for predicting Tc,max of hole-doped cuprates using material-dependent parameters as features, whose relation to Tc,max has been reported. We select four features, including the Bader charge of apical oxygen, the bond strength between apical atoms, the number of superconducting layers, and the apical oxygen height. The features are easily accessible from first-principles calculations and experimental crystal structures. To reveal a direct connection between the four features and the target variable, Tc,max, we search for explicit analytical equations by applying the linear regression with nonlinear functional forms by the brute force searching (BFS) algorithm. The non-parametric RF is also employed to analyze the quantitative contribution of each feature to the output. Our model is distinguished from the previous ML models on the Tc prediction by using the material-dependent parameters beyond simple composition features and providing an explicit functional form with features for high Tc cuprates. Furthermore, we generate hypothetical cuprates by changing the apical cation and predict the corresponding Tc,max based on the developed BFS model. The cuprate with Ga as an apical cation is predicted to exhibit Tc,max comparable to that of the Hg-family.

The workflow of this work is shown in Figure 1. All density functional theory calculations were performed with the Vienna Ab Initio Simulation Package (VASP). The PAW–PBE functional was employed for the exchange–correlation functional. We performed nonspin polarized calculations with U = 8 eV and J = 1.34 eV for the Cu d orbitals and with a 520 eV plane-wave energy cutoff. We used the four features of 29 hole-doped cuprates, which have been reported as material-dependent parameters: the Bader charge of the apical oxygen (B), the apical force (F), the number of CuO2 layers (L), and apical oxygen height (da). Computational details and data acquisition are in the Supporting Information.

We employed two machine learning algorithms: one is a parametric BFS model, and the other is a nonparametric RF regression. To avoid overfitting, we evaluated the performance of each model using leave-one-out cross-validation (LOOCV) unless specified otherwise. The BFS model is a linear regression with various functions converting primary features to the nonlinear functional forms of compound features. We have four primary features (B, Fa, L, and da) and 15 functions (1, x, 1/x, x^2, 1/x^2, x^3, 1/x^3, 1/ln(x+1)), 1/ln(x+1), ln(x+1), and ln(x+1)), which produce 57 distinct prototypical features. Multiplication of these prototypical features taking two, three, or four generates 50 625 compound features. The compound features are used to construct linear regression models in the form of Tc,max = θ0 + Σm=1 θm f m, where θ0, f m, and m represent the regression coefficients, compound features, and the total

Figure 1. Schematic workflow of the ML prediction models for Tc,max of hole-doped cuprates.
number of compound features, respectively. We define the mCnF model as a linear regression model with m compound features where each compound feature consists of n primary features. Note that each compound feature in an mCnF model can have different n primary features. One example of a 3C2F model is

\[ \theta \theta \theta + + FL d 01 e e 21 e B L L A 1/ A. \]

We searched for the best BFS fit using all data as a training set and evaluated the three best-fit BFS models for each case using the LOOCV. On the other hand, the RF method is one of the most widely used ML algorithms because of its simplicity and ability to learn nonlinear dependencies. Especially, the RF provides the importance of each feature, the so-called Gini importance (GI). Details of machine learning algorithms are in the Supporting Information.

Figure 2a,b shows the performance of BFS models for predicting \( T_{c,\text{max}} \) depending on the number of primary features and compound features. (c) Comparison of the experimental \( T_{c,\text{max}} \) against the predicted \( T_{c,\text{max}} \) obtained by the best 3C2F model. (d) The shape of the equation of the BFS model with the smallest RMSE of 3.705 K. The color bar indicates the calculated \( T_{c,\text{max}} \).

Table 1. Details of Model Equations of the Best Three 3C2F Models for Prediction of \( T_{c,\text{max}} \)

| Model | Equations | RMSE (K) | \( R^2 \) |
|-------|-----------|----------|---------|
| 1     | \[ 96.3 - 0.789 \frac{\theta}{\varepsilon^2} + 689 \frac{1}{\beta/{\lambda}^2} - 348 \frac{1}{\varepsilon^2} \] | 3.705 (4.609) | 0.969 (0.956) |
| 2     | \[ -21.6 + 307 \frac{\theta}{\varepsilon^2} - 611 \frac{1}{\beta/{\lambda}^2} + 58.1 \frac{1}{\varepsilon^2} \] | 3.795 (4.840) | 0.957 (0.942) |
| 3     | \[ -19.1 - 0.705 \frac{\theta}{\varepsilon^2} + 240 \frac{1}{\beta/{\lambda}^2} + 327 \frac{1}{\varepsilon^2} \ln(1 + 10\varepsilon) \] | 4.197 (4.843) | 0.955 (0.953) |

\( F_A, B, \text{ and } L \) represent the apical force, the Bader charge of the apical oxygen, and the number of CuO2 layers, respectively. The numbers in parentheses are from 5-fold CV.

The best three BFS models for the 3C2F are summarized in Table 1, showing the empirical equation to predict the \( T_{c,\text{max}} \) of cuprates. The best three models exhibit similar prediction performances according to the RMSE and \( R^2 \). We have also tested the 5-fold CV, and the RMSE and \( R^2 \) with 5-fold CV are similar to those of LOOCV as in Table 1. In addition, to further investigate the predictability of the BFS models, we have performed forward 5-fold CV, where the data set is sorted by \( T_{c,\text{max}} \) values before doing 5-fold CV. The RMSEs of the best three BFS models under the forward 5-fold CV are 5.101 K.
K (model 1), 5.727 K (model 2), and 5.645 K (model 3), which are comparable with the results using the 5-fold CV and LOOCV. The similar performance results among different CV methods suggest the predictability of our BFS models.

The complicated equation with functionals such as \( e^x \sqrt{x} \) and \( \ln(x+1) \) in Table 1 indicates the nonlinear relationship between features and \( T_{c,max} \). Interestingly, the apical oxygen height (\( d_A \)) feature does not appear in the best three, which implies that the \( d_A \) is less important than other features of Bader charge of the apical oxygen (\( B \)), apical force (\( F_A \)), and the number of CuO2 layers (\( L \)). Although the interpretation of equations is not straightforward, our ML model provides the quantitative relation with \( T_{c,max} \) and expands previous qualitative correlation of the physical parameters, which are related to lattice dynamics of the apical oxygen and apical charge flux. It is worth noting that the \( T_{c,max} \) of cuprates can be predicted using these analytic functional forms with high accuracy, which needs only the readily available three material-dependent parameters.

To investigate the relationship between primary features and \( T_{c,max} \), we illustrated the shape of the equation of the best 3C2F model with parameters of \( B, F_A, \) and \( L \), as shown in Figure 2d. It shows that, for example, a material with \( (B, F_A, L) = (7.3, 2.0, 2) \) expects to have a \( T_{c,max} \) of 104 K. Despite the different equation forms, the three equations exhibit a similar shape as in Figure S1, and their general shapes have the common characteristics that (i) the predicted \( T_{c,max} \) increases as \( B \) decreases, (ii) predicted \( T_{c,max} \) increases as \( F_A \) increases, and (iii) the predicted \( T_{c,max} \) has the maximum around \( L \) of 3 or 4, which are consistent with the previous papers. Our BFS model thus properly captures the expected relationship between each feature and \( T_{c,max} \).

We have performed the nonparametric RF regression model, which can learn complicated nonlinearity, to further investigate the importance of each feature to \( T_{c,max} \). Figure 3a shows the performance of the RF depending on the number of features. Each point was obtained from the feature combination with the smallest RMSE. When using only two features, \( B \) and \( L \), the RF model exhibits the best performance with the RMSE of 7.735 K and \( R^2 \) of 0.837, as shown in Figure 3b. Under 5-fold CV, the RMSE and \( R^2 \) using \( B \) and \( L \) features are 9.714 K and 0.804, respectively, which are similar to those with the LOOCV. The second-best RF model has the RMSE of 9.196 K and \( R^2 \) of 0.731 with three features of \( B, L \), and \( F_A \). The performance of the RF model is not better than the BFS model but shows a reasonable accuracy. Furthermore, we have explored the RF model with all the 50 625 compound features and three major compound features, \( \frac{e^x}{\sqrt{x}}, \frac{1}{\sqrt{F_A}}, \) and \( \frac{e^{x/L}}{e^{x}} \) in the best 3C2F model. Note that the three compound features are generated from the three primary features, \( B, L \), and \( F_A \). The RMSE and \( R^2 \) using all the compound features are 9.460 K and 0.741, and those with the three compound features are 9.704 K and 0.723, which are similar to those using the three primary features. This result indicates that the RF itself can deal with complex nonlinear dependencies of the data.

Table 2 represents the Gini importance (GI), which measures feature relevance on the output parameter, in our case, \( T_{c,max} \). The GI for \( B \) and \( L \) in the best RF model are 0.555 and 0.445, respectively, which implies a similar contribution of \( B \) and \( L \) to predict \( T_{c,max} \). In the second-best RF model, \( B \) and \( L \) exhibit a slightly larger GI than that of \( F_A \), but all three have a similar GI of ~0.3. These results suggest that \( B \) and \( L \) are the most important features to predict \( T_{c,max} \) followed by \( F_A, d_A \) would be the least important feature among them. The high GI of the Bader charge \( B \) of apical oxygen here may also be related to the charge flux discussions regarding the transport property and pseudogap phase.

Note that the parametric model and the nonparametric model have their own advantages. The parametric BFS model provides high accuracy as well as analytical and explicit formulas for \( T_{c,max} \) which cannot be obtained from the RF model because of its implicit regression process. The nonparametric RF algorithm has advantages of low computational cost and reasonable predictability, in our case, with only two simple features. In addition, the RF model provides the quantitative feature importance.

We further investigate the correlation not only between a feature and \( T_{c,max} \) but also among features using the Pearson correlation coefficient, \( r_{xy} \). The Pearson correlation coefficient is defined as

\[
r_{xy} = \frac{\sum_{i=1}^{m} (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{m} (x_i - \bar{x})^2} \sqrt{\sum_{i=1}^{m} (y_i - \bar{y})^2}}
\]

where \( x_i \) and \( y_i \) are parameters indexed with \( i \) among the total data size, \( m \). The upper bar indicates the average. The Pearson
correlation coefficient shows the strength of linear correlation between two parameters in a range of −1 to 1. When the coefficient is close to 1, a strong correlation is indicated.

Figure 4 shows the Pearson correlation map for the features and $T_{c,\text{max}}$. B, $F_A$, and L have a strong correlation with $T_{c,\text{max}}$.

![Figure 4](image-url)

**Figure 4.** Correlation map of the features and $T_{c,\text{max}}$ by the absolute values of the Pearson correlation coefficient.

with the coefficient $\geq 0.59$, which is consistent with our BFS, RF model, and GI importance. B and L have the least correlation, which explains reasonable accuracy in the RF model using only B and L. We also can see $F_A$ is highly correlated with $d_A$ exhibiting the coefficient of 0.87, which explains the high predictability even without the $d_A$ feature. In addition, the coefficient between $F_A$ and $T_{c,\text{max}}$ (0.63) is larger than that of $d_A$ and $T_{c,\text{max}}$ (0.48), which suggests that, if we have to choose one feature between of $F_A$ and $d_A$, $F_A$ would be the better choice.

To search for a new cuprate candidate, we have generated hypothetical structures by replacing apical cations with other elements. Considering the HgBa$_2$CaCu$_2$O$_y$ (Hg-1212) structure, we changed the Hg atom with alkali-earth elements (Mg, Ca, Sr, Ba), elements in groups 11–15 and in periods 4–6. Figure 5 shows the average of predicted $T_{c,\text{max}}$ of the best three 3C2F models for hypothetical structures, compared with the experimental $T_{c,\text{max}}$ for YBa$_2$Cu$_3$O$_7$ (group 11, period 4), Hg-1212 (group 12, period 6), Tl$_2$Ba$_2$CaCu$_2$O$_y$ (group 13, period 6), and Pb$_2$Sr$_2$YCu$_3$O$_y$ (group 14, period 6). For periods 5 and 6, $T_{c,\text{max}}$ is a maximum with the group 12 elements as the apical cation. For period 4, $T_{c,\text{max}}$ is the highest with the group 13 element. Ga. Figure S3 shows the predicted $T_{c,\text{max}}$ using the BFS 2C3F model. Even though the estimated values are slightly different from those of the 3C2F model, a similar trend shows the robustness of the prediction (see Figure S3).

We have investigated the Ga case, GaBa$_2$CaCu$_2$O$_y$ (Ga-1212), which has the highest $T_{c,\text{max}}$ among hypothetical structures, and a predicted $T_{c,\text{max}}$ comparable to that of Hg-1212. The apical force and the Bader charge of Ga-1212 are 1.73 eV/Å and 7.20, while those of Hg-1212 are 1.66 eV/Å and 7.13, respectively. With the help of ML, the $T_{c,\text{max}}$ values of new structures are quantitatively estimated; otherwise, we can only speculate that Ga as the apical cation might have a chance to exhibit high $T_{c,\text{max}}$. We further generated and predicted the $T_{c,\text{max}}$ of GaBa$_2$Ca$_{n+1}$Cu$_2$O$_{2n+4}$ (Ga-12(n−1)n, n = 1, 2, and 3) and GaBa$_2$Ca$_{n+1}$Cu$_2$O$_{2n+4}$ (Ga-22(n−1)n) as shown in Table 3. The base structure for the latter case is Tl$_2$Ba$_2$Ca$_{n+1}$Cu$_2$O$_{2n+4}$.

**Table 3.** Predicted $T_{c,\text{max}}$ of Ga-12(n−1)n and Ga-22(n−1)n Compared with Experimental $T_{c,\text{max}}$ of Hg-12(n−1)n*

| n  | Ga-12(n−1)n (K) | Ga-22(n−1)n (K) | Hg-12(n−1)n (K) |
|----|----------------|----------------|-----------------|
| 1  | 71             | 107            | 94              |
| 2  | 117            | 142            | 127             |
| 3  | 131            | 152            | 135             |

* $n$ indicates the number of CuO$_2$ layers.

(Tl-22(n−1)n). The calculated $T_{c,\text{max}}$ for Ga-22(n−1)n is higher than those of Ga-12(n−1)n. The B of Ga-22(n−1)n and Ga-12(n−1)n are similar, while the $F_A$ of Ga-22(n−1)n, $\sim$1.71 eV/Å, is greater than that of Ga-12(n−1)n, $\sim$1.73 eV/Å, which results in the greater $T_{c,\text{max}}$ of Ga-22(n−1)n. A few experimental studies reported the $T_c$ of cuprates having Ga as an apical anion (GaSr$_2$Ca$_{n-1}$Cu$_2$O$_{2n+3}$ type) whose $T_c$ are reasonably high as 49–68, 70–73, and 107 K for $n = 2, 3,$ and 4, respectively. It would be worth revisiting the Ga family with GaBa$_2$Ca$_{n-1}$Cu$_2$O$_{2n+2}$ type or GaBa$_2$Ca$_{n-1}$Cu$_2$O$_{2n+4}$ type structures, because our predictions show a higher $T_{c,\text{max}}$ in these two types.

In conclusion, we have developed machine learning models using the BFS and RF algorithms for predicting $T_{c,\text{max}}$ of hole-doped cuprates. To improve the physical interpretability of the models, we used four readily accessible material-dependent parameters for $T_{c,\text{max}}$, namely the DFT calculations ($F_A$ and B) and structural experiments ($L$ and $d_A$). The BFS model provides the empirical and explicit equation with three parameters, B, L, and $F_A$, for $T_{c,\text{max}}$, which exhibits high accuracy of the RMSE of 3.705 K and $R^2$ of 0.989. The RF model shows the reasonable accuracy of the RMSE of 7.735 K and $R^2$ of 0.837 using only two features of B and L. By analyzing the BFS results, the GI importance, and Pearson’s correlation coefficient, we found that B, L, and $F_A$ are important to predict $T_{c,\text{max}}$ which implies the role of apical oxygen phonon and apical charge flux in $T_{c,\text{max}}$. Furthermore, we predicted the $T_{c,\text{max}}$ of hypothetical structures where the Hg atom is replaced with other elements. When Ga is the apical cation, the $T_{c,\text{max}}$ values are the highest with 71, 117, and 131 K for one, two, and three CuO$_2$ layers, respectively. We hope that this work can inspire the theoretical development of the $T_c$
equation and guide the experimental search for new cuprate superconductors.

**ASSOCIATED CONTENT**

- Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.jpcl.1c01442.

Detailed computational and machine learning methods, summary of \( T_{c,max} \) and \( d_{\alpha} \) of materials, shape of the equations in the 3C2F model, results of the 2C3F model, and predicted \( T_{c,max} \) of hypothetical structures in the 2C3F model (PDF)

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**Notes**

The authors declare no competing financial interest.

**ACKNOWLEDGMENTS**

We thank Hyungchul Kim and Xi Chen for helpful discussions. This work was supported by the National Research Foundation of Korea (NRF) (Grant 2019R1F1A1052026) and Korea Electric Power Corporation (Grant R20XO02-12).

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