

Prediction of ferroelectric properties of (K,Na)NbO₃-based solid solutions with the aid of interpretable descriptors

Tatiana S. Ilina¹, Sofia V. Torianik¹, Dmitrii S. Zakhidov¹, Dmitry A. Kiselev¹

1 National University of Science and Technology "MISIS", 4-1 Leninskiy Ave., Moscow 119049, Russian Federation

Corresponding author: Sofia V. Torianik (torianiksofia@gmail.com)

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Abstract

This work puts forward an interpretable approach for predicting ferroelectric properties on the basis of sure independence screening and sparsifying operator (SISSO) method, which uses a symbol regression for studying mathematically compact expressions having explicit physical sense. In combination with ensemble machine learning (ML) methods, i.e., extra trees regressor (ETR), random forest (RF), gradient boosting regressor (GBR), and extreme gradient boosting (XGBoost), as well as SHAP (SHapley Additive exPlanations) analysis for the selection and interpretation of features, the approach developed in this work simultaneously delivers high prediction accuracy and possibility to study fundamental mechanisms underlying the formation of ferroelectric properties in materials. Based on the available experimental data for 476 potassium-sodium niobate (KNN-based) ceramic specimens, feature engineering has been carried out, as a result of which the key physical descriptors have been separated and the optimal choice of predictors has been determined. The model developed herein allows explicit, i.e., in a formularized form, description of quantitative relationships between structural parameters and functional characteristics of materials. The methodological approach to interpretable machine learning put forward in this work opens up new possibilities for the optimization-driven design of piezoelectric ceramics and other functional materials, and will be useful both for fundamental research and practical applications.

Keywords

KNN ceramics, ferroelectric properties, machine learning, sure independence screening and sparsifying operator

1. Introduction

The development of lead-free KNN-based piezoceramics has become one of the most rapidly growing trends of materials science in recent decades due to their high piezoelectric response and environmental friendliness [1, 2]. The search for new functional materials has been conventionally based on an extremely difficult empirical approach [3]. Despite the multiple discoveries that

approach has led to, it detracts from significant limitations, most clearly expressed in the current epoch of growing complexity of multicomponent material compositions and the requirement to minimize the time of their implementation [3–5]. Since the path from a fundamental understanding to a commercial product can take decades [6], accelerated search for material compositions and optimization methods acquire special importance.

One of the most promising tools to solve the above task is machine learning (ML). The implementation of ML methods gives new opportunities in materials science for accelerated search for compositions with preset characteristics and retrieval of latent regularities in the “composition – structure – properties” system [7]. Machine learning models can analyse large datasets, identify non-linear relationships between the composition and properties of materials, and predict, with a high precision, the parameters of new, yet not synthesised compounds [7]. Such methods are already successfully used for the prediction of extended properties, including piezoelectric coefficients [8], Curie temperatures [9], and piezoelectric permittivity [10]. Of special interest are lead-free KNN-based piezoelectric materials, which are considered as an environmental-friendly alternative to noxious lead zirconate-titanate-based materials [11, 12]. Chemical modification through complex multicomponent doping is the key method to improve the piezoelectric properties [2], yet it leads to an exponential growth of the number of possible composition combinations, thus making them ideal for ML applications [13].

Despite the high predictive capability, most of the existing ML models, such as deep neural networks or complex ensemble methods, often operate by the “black box” principle, which limits their application in materials science [14]. The lack of interpretability complicates the understanding of latent mechanisms determining the properties of materials and undermines confidence to the predictions [15]. Therefore increasing attention is paid to the application of interpretable models.

One of the most powerful tools to develop interpretable models is the use of symbolic regression, e.g. the sure independence screening and sparsifying operator (SISSO) method [16]. Sure independence screening and sparsifying operator allows identifying compact analytical descriptors which directly associate the fundamental properties of elements with the target property, thus delivering a high degree of interpretability. For example, not only the piezoelectric coefficient d_{33} of KNN-based ceramics was successfully predicted using SISSO, but also an interpretable descriptor was suggested which correlates with phase transition mechanisms underlying the high piezoelectric response of materials [8]. In another work, SISSO allowed identifying the key role of covalent and Van-der-Vaals radii of B-cations in the ABO_3 perovskite structure in the determination of the d_{33} of KNN, with an error of ~ 40 pC/N [17].

Along with interpretable methods, e.g. SISSO, prediction accuracy is maximized in case of wide application of ensemble machine learning methods, including extra trees regressor (ETR), random forest (RF), gradient boosting regressor (GBR), and extreme gradient boosting (XGBoost). For example, the ETR model with an optimum set of seven features allowed predicting the d_{33} of KNN with an error of ~ 49 pC/N [8]. Active learning based on ML models also showed its efficiency in the

synthesis of a KNN composition with $d_{33} \sim 353$ pC/N, which is far above the respective figures of most specimens in the initial training set [13]. Importantly, the efficiency of models depends on the correct choice of features. Studies show that such characteristics as electronegativity, ratio between the number of valence electrons and the nominal charge, and electron core radius (by Schubert) are the key ones not only for the prediction of the piezoelectric properties of KNN, but also for the classification of perovskites into ferro- and antiferroelectrics [4].

Despite the above achievements, most works are focused on the prediction of a single feature, typically, d_{33} , whereas the practical application of materials requires a set of characteristics be known, e.g. the piezoelectric coefficient, the Curie temperature T_C , and the dielectric permittivity ϵ .

The aim of this work is system analysis and comparing the efficiency of ensemble machine learning algorithms (RF, ETR, XGBoost, and GBR) in predicting the three key properties of lead-free KNN-based piezoelectric ceramics: the piezoelectric coefficient d_{33} , the Curie temperature T_C , and the dielectric permittivity ϵ . The work will also deal with comparison between the models for prediction accuracy, retrieval of physically meaning regularities using SISSO in combination with SHAP, and validation of the modeling results against experimental data borrowed from literature.

2. Methodology

The target properties for this work were the piezoelectric coefficient (d_{33}), the dielectric permittivity at room temperature measured at a frequency of 10 kHz (ϵ), and the Curie temperature (T_C).

2.1. Database

In this work, the dataset includes 476 KNN-based ceramic specimens [18–83] containing information on the chemical composition, the piezoelectric coefficient (d_{33}), the Curie temperature (T_C), and the dielectric permittivity (ϵ), as well as 22 initial fundamental features presented in Table 1. In the works [8, 84, 85] it was established that these initial features provide high-quality predictions of ferroelectric properties. In order to provide data accuracy and consistency, only solid-state sintered specimens were included in the dataset.

2.2. Calculation of parameters

For each composition, the initial features summarized in Table 1 were calculated. The fundamental features of the chemical elements (effective ionic radii, volume of atom, etc.) were obtained from the literature and open sources [86–89]. As a result, a set of initial features were obtained

Table 1. Initial features

	A-site	B-site	Reference
Effective ionic radii	r_A	r_B	[86]
t is tolerance factor	$t = \frac{r_A + r_O}{\sqrt{2} (r_B + r_O)}$		[87]
μ is octahedral factor	$\mu = r_B/r_O$		
Volume of atom	V_A	V_B	[88]
Atomic weight	AW_A	AW_B	
Effective nuclear charge (Slater)	NC_A	NC_B	
Distance from core electron (Schubert)	DCE_A	DCE_B	
Distance from valence electron (Schubert)	DVE_A	DVE_B	
Electron affinity	EA_A	EA_B	
Nuclear magnetic moment	MN_A	MN_B	
Valence electron number	NV_A	NV_B	
Electronegativity (Pauling)	EN_A	EN_B	[89]

which were calculated as values X (see Table 1) separately for the A- and B-sites of the perovskite structure, in accordance with the following formulas:

$$X_A = \sum_{i=1}^n f_i X_{Ai}, \quad (1)$$

$$X_B = \sum_{i=1}^n f_i X_{Bi}, \quad (2)$$

where n is the number of atoms in the A/B-sites of the perovskite structure and f_i is the atomic fraction of each of the ions.

2.3. SISO

At the first stage, the dataset with a set of required fundamental features were used for obtaining interpretable descriptors using SISO. This allowed not only to increase the accuracy of prediction due to the use of the models, but also to preserve their physical interpretability. Unlike the direct use of regression models, we used a two-stage feature selection strategy for reducing the dimension of the initial space of descriptors obtained using SISO and excluding multicollinearity which deleteriously affects the calculative efficiency of the models.

2.4. Feature selection

The resultant set of 500 SISO descriptors for each of the three target properties (d_{33} , T_C , and ϵ) were ranged by the degree of mutual interrelation and correlation with the target property. The descriptors weakly correlating with the target property (Pearson correlation coefficient <0.1) and the strongly mutually interrelating ones (Pearson correlation coefficient >0.7) were excluded. Then, 20 descriptors remained that were weakly correlated with each other and well correlated with the target property.

For the remaining 20 most relevant descriptors, their effects on the predictive capacity of the models were quantitatively characterized using the mutual information (MI). Mutual information allows one to evaluate the relationships between the descriptors and the target property, which is of special importance for analysis of complex physical properties of ferroelectrics. As a result of analysis, seven most meaning descriptors for each of the three target properties were selected for further learning.

2.5. Machine learning methods

The seven most meaning descriptors generated with SISO were used for further modeling using ensemble machine learning algorithms, e.g. RF, ETR, XGBoost, and GBR.

The resultant machine learning models were interpreted for the final set of descriptors using the SHAP method (SHapley Additive exPlanations). This approach allows quantitative characterization the importance of each feature for the overall prediction. SHAP analysis of features allows ranging the descriptors by the degrees of their physical meaning, which is important for meaningful verification of the models from the standpoints of process physics.

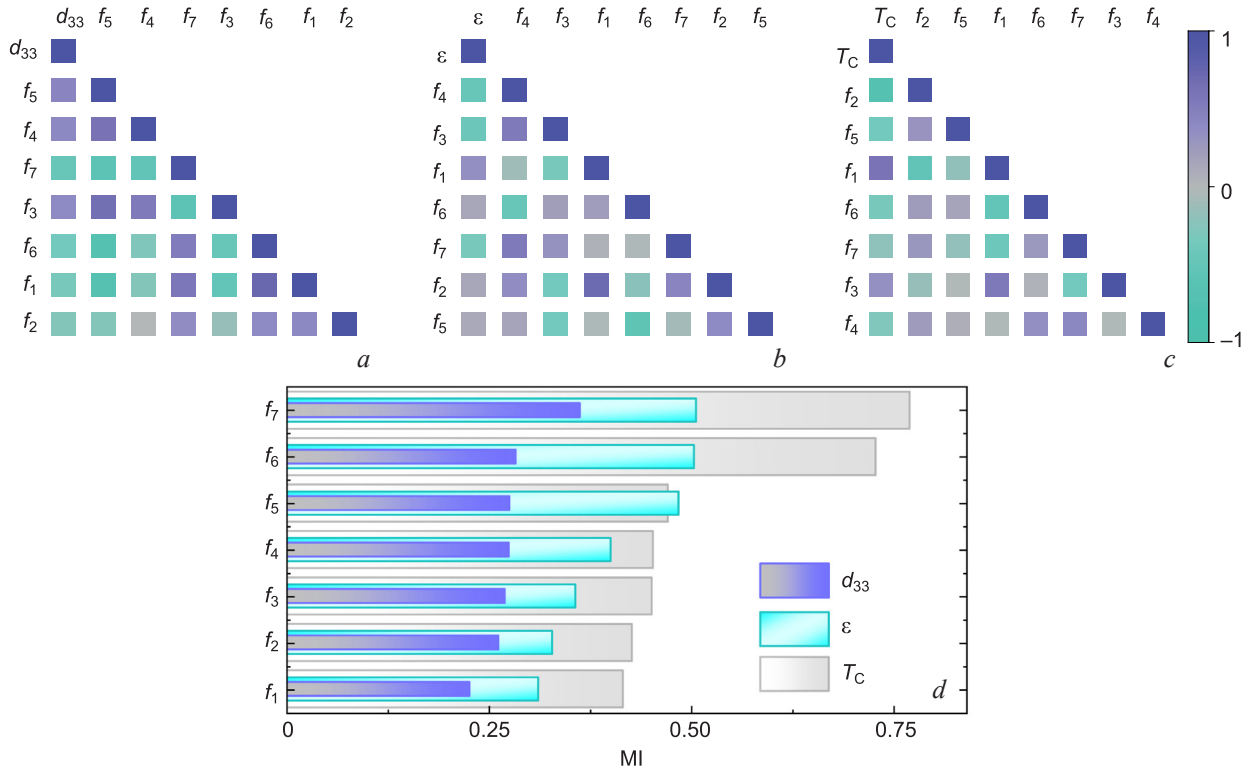
3. Results

3.1. Pearson method and mutual information

For each target property, the dataset included more than 200 experimental values. As noted above, 7 most informative descriptors were selected for each parameter at the feature selection stage. The final set of descriptors used for the machine learning models is summarized in Table 2.

Table 2. SISSO descriptors

d_{33}	ε	T_C
$f_1 = (EA_A - AW_A)(t - EN_A)$	$f_1 = 1/(EN_B - V_B)$	$f_1 = (V_B - NV_A)(r_B - NV_A)$
$f_2 = (NV_B - MN_B)^2$	$f_2 = MN_B \times EA_B \times (DCE_B - DCE_A)$	$f_2 = DCE_B \times V_B + (DCE_B - DCE_A)$
$f_3 = EA_A \times NC_A \times \sqrt{EA_B}$	$f_3 = MN_B \times DCE_A \times (NV_B - V_B)$	$f_3 = (V_A - AW_A)(MN_B - NV_A)$
$f_4 = MN_B \times MN_A \times (DVE_B - DCE_A)$	$f_4 = \mu \times MN_A + (MN_B - r_A)$	$f_4 = r_A^2 - \mu \times V_A$
$f_5 = MN_B \times AW_A \times (DVE_B - DCE_A)$	$f_5 = EN_B + V_A - \sqrt{AW_B}$	$f_5 = (DVE_B - DCE_A) \times (DCE_B - DCE_A)$
$f_6 = EN_A \times NV_A + (NV_B - NV_A)$	$f_6 = (EN_B + EN_A) - (MN_B + NV_A)$	$f_6 = MN_A \times AW_A \times (NC_B - NC_A)$
$f_7 = (EN_B - V_B) \times (MN_B - V_B)$	$f_7 = NV_B - EN_A - \sqrt{EA_B}$	$f_7 = NC_B \times r_A \times t \times EA_A$

**Figure 1.** Pearson correlation matrix for set of features for (a) d_{33} , (b) ε , (c) T_C , and (d) MI for SISSO descriptors

Figures 1a–1c shows the Pearson correlation matrices for the final sets of seven descriptors used for d_{33} , ε , and T_C prediction. Analysis of the matrices confirmed the absence of high pairwise correlation between the selected descriptors, suggesting that each of the descriptors bears unique information on the properties of the material, without information duplication in other descriptors.

The descriptor meaning charts obtained using the MI method are shown in Fig. 1d. Analysis of these graphs suggests that all the selected descriptors have sufficient predictive capability and are highly important for the prediction of the target properties. The absence of descriptors with negligibly low MI values confirms that each feature is informative and not excessive, and their combination provides for the maximally complete description of the “composition – property” interrelationships.

Pearson and MI analyses of the descriptors suggest that the generated set of descriptors is optimal, balanced, and free from multicollinearity and non-informative features.

3.2. Model evaluation

The initial data were divided into the training and test sets in a 80/20 ratio. Four machine learning models were selected for the prediction of the properties of KNN-based ceramics: ETR, RF, GBR, and XGBoost. The learning of each model for d_{33} , ε , and T_C prediction was carried out independently, using the respective sets of 7 descriptors. The performance of the learnt models was evaluated based on the determination coefficients (R^2) of the training and test sets.

Model performance evaluation results are presented in Fig. 2, showing the dependence of predicted values on

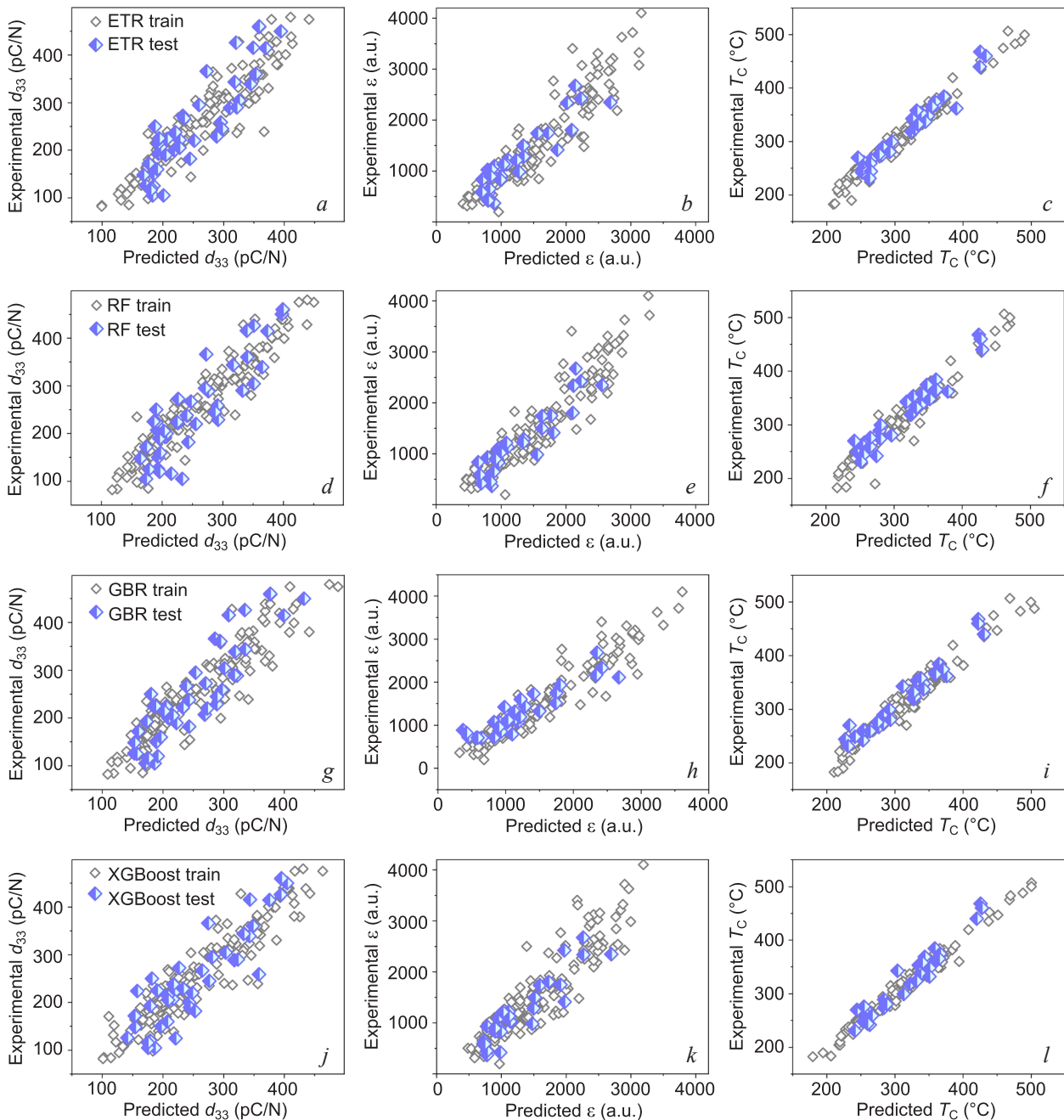


Figure 2. Performance of ML models: (a–c) ETR, (d–f) RF, (g–i) GBR, and (j–l) XGBoost in prediction of (a, d, g, j) d_{33} , (b, e, h, k) ϵ , and (c, f, i, l) T_c for KNN-based ceramics

experimental ones for each of the four models and three target properties.

The proximity of the data points to the perfect fit lines in the diagrams confirms good predictive capability of the algorithms tested. Quantitative comparison between the models is presented in the form of bar charts (Fig. 3) illustrating the R^2 values.

3.3. Validation

A final check of the predictive capability of the models was carried out for independent correlation sets containing 10 compositions each, for each target property.

The validation sets for d_{33} , ϵ , and T_c are presented in Supplementary Information.

Comparison between the predicted and experimental values for the validation data is shown in Fig. 4. The average relative errors of prediction for each model and each target property are summarized in Table 3 and prove to be within limits that allow using the test models for the development of new compositions with tailored properties.

Based on the preliminary analysis of the four machine learning models tested for each of the three target properties, algorithms were selected which were the most suitable for the prediction of respective properties. The ETR

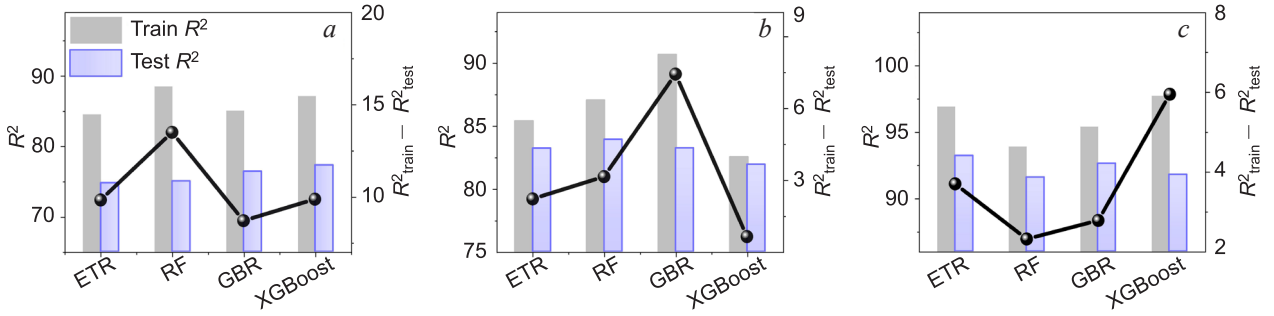


Figure 3. Analysis of ML models performance in prediction of (a) d_{33} , (b) ϵ , and (c) T_C for KNN-based ceramics

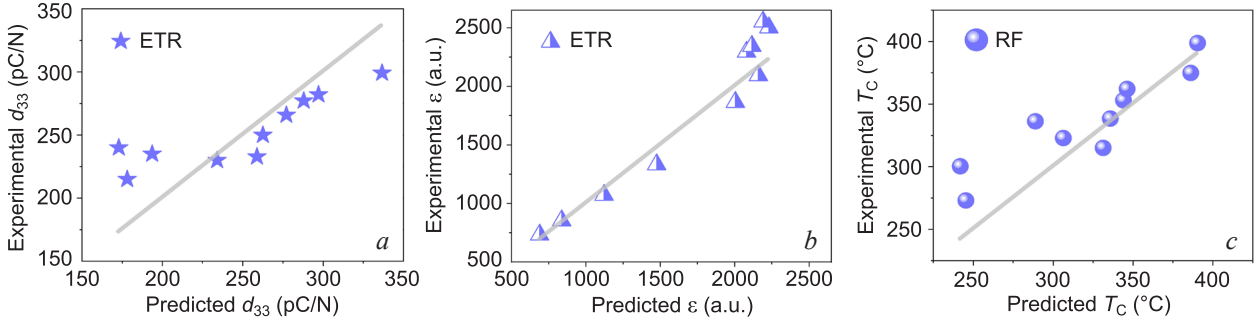


Figure 4. Validation of ML models: (a) ETR for d_{33} , (b) ETR for ϵ , and (c) RF for T_C for independent experimental data borrowed from literature

model is the optimum one for the prediction of piezoelectric coefficient, since it showed the least average relative error for its independent validation set (10.7 %) combined with competitive R^2 for the test set (75 %). Prediction of dielectric permittivity is also best done using the ETR model which showed the smallest error for the validation data (7.8 %) and stable R^2 values for the test set (83 %). The RF model proved to be the most effective in predicting the Curie temperature due to the smallest average relative error (6.7 %) for the validation set, while retaining high R^2 (91 %).

4. Discussion

The key tool of machine learning model interpretation is to evaluate the contribution of individual features, and this was implemented in this work using the SHAP method. Figure 5 shows SHAP values for descriptors illustrating the degree of their impact on the prediction of the three target properties using the optimal models which demonstrated the highest accuracy.

For interpretable machine learning in the analysis of KNN-based ceramic materials, the key result is the identification of the descriptors which have the lowest SHAP values, indicating their predominant impact on the prediction of the target properties.

A significant impact of the descriptor $f_2 = (NV_B - MN_B)^2$ on the predicted piezoelectric coefficient d_{33} can be accounted for by the physical nature of the parameter MN_B (nuclear magnetic moment of the B-cations in ABO_3 -type perovskite structures). The parameter MN_B exerts a strong impact on the value of d_{33} , since it is an

Table 3. Average relative error of ETR, RF, GBR, and XGBoost models in prediction of d_{33} , ϵ , and T_C

Model	Average relative error (%)		
	d_{33}	ϵ	T_C
ETR	10.7	7.8	7.8
RF	13.0	8.1	6.7
GBR	13.5	11.8	8.4
XGBoost	14.7	9.4	6.8

effective indicator which integrates the electron configuration and crystal structure that determine the piezoelectric response of materials [8]. According to earlier works, local ferroelectric distortions induced by dopants at the B-sites directly determine Landau's local energy barrier, thus critically affecting polarization and switching under external electric fields [90, 91]. The parameter MN_B correlates with the electronegativity and hybridization degree of the d -orbitals of the ions at the B-sites with $2p$ -orbitals of the surrounding oxygen atoms, this controlling the rigidity of the chemical bonds and the mobility of the ion in the oxygen cluster [11].

The greatest impact on the prediction of dielectric permittivity comes from the descriptor $f_4 = \mu \times MN_A + (MN_B - r_A)$. The component μ is the octahedral factor determining the geometry of the oxygen octahedron BO_6 . According to classical standpoints [86], the ratio of the ionic radii of B and O affects the distortion degree of the octahedrons. The expression $\mu \times MN_A$ describes the relationship between the geometry and the electron configuration of the atoms the A-sites (volume and effective radii: the nuclear magnetic moment MN_A correlates

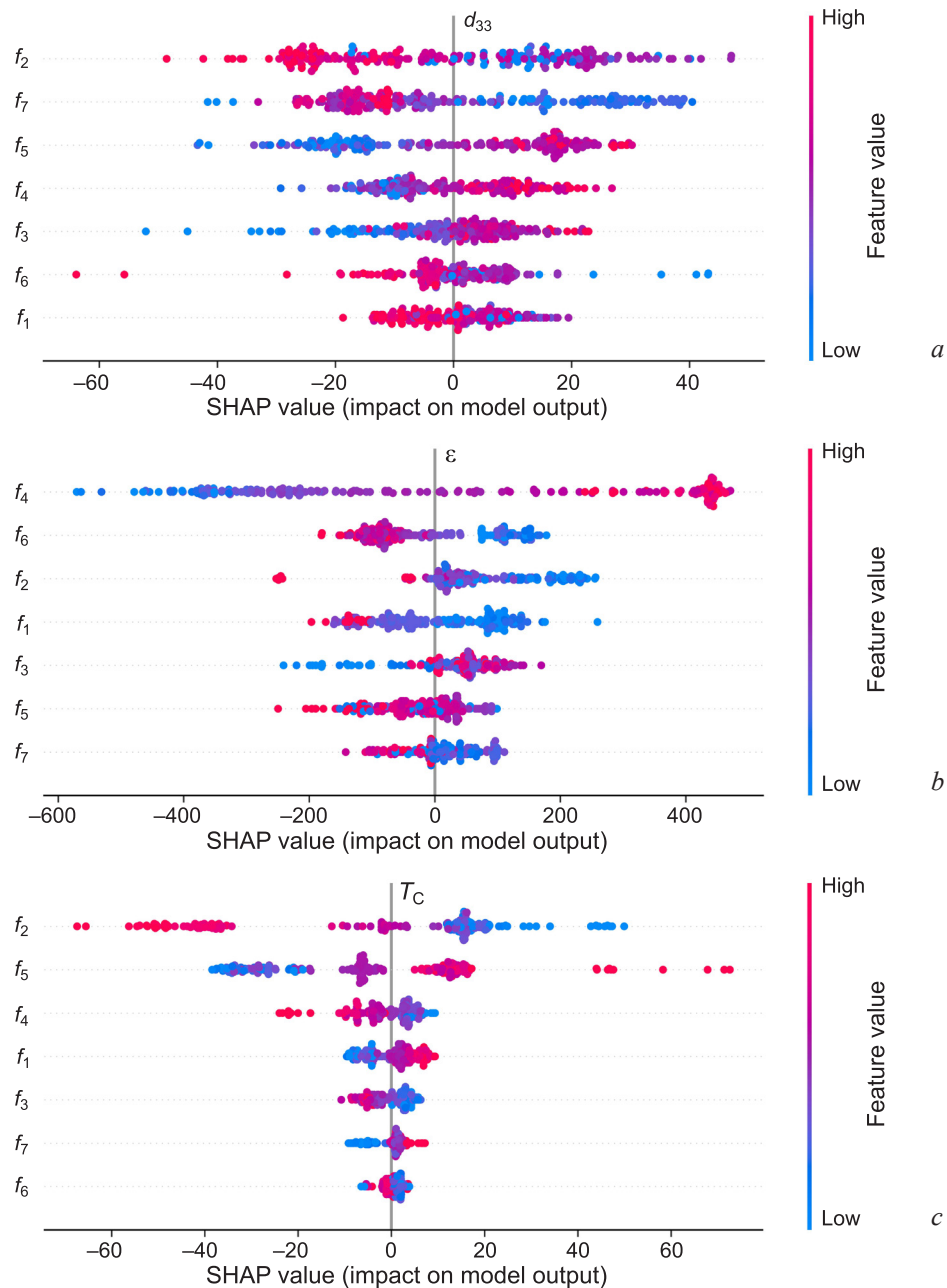


Figure 5. SHAP-based analysis of impact of features on predictive capability of models: (a) ETR for d_{33} , (b) ETR for ϵ , and (c) RF for T_C

with the electronegativity and polarizability of the ions in the A-sublattice, hence determining the contribution of electron polarization [8]. The expression $(MN_B - r_A)$ shows the interaction between the electron configuration of the B-cations and the dimensional factor of the A-cations. As shown earlier [8], MN_B is important for the description and prediction of d_{33} (this is, accordingly, related to the value of polarization), while the ionic radius r_A controls the free space left for ionic shifts, which is of special importance for phase transitions [92]. An increase in the polarizability of the B-cation (large MN_B) acts to increase the electronic and ionic polarization. Optimization of the octahedron geometry ($\mu \rightarrow 1$) decreases the energy barrier for ionic shifts. Achievement of a balance between the A-cation size and the electron configuration

of the B-site favors the formation of morphotropic phase boundaries (orthorhombic-tetragonal, rhombohedral-orthorhombic, rhombohedral-tetragonal), leading to high dielectric responses [92]. Thus, the descriptor f_4 covers the multicomponent nature of dielectric response: electronic polarization (MN_A , MN_B), ionic polarization in phase transition regions (μ , lattice distortions).

Analysis of SHAP values allowed to highlight the descriptor $f_2 = DCE_B \times V_B + (DCE_B - DCE_A)$, which integrates the electron configuration and geometric parameters of atoms determining the Curie temperature (T_C) of KNN-based ceramics. The validity of using the above-listed atomic features was additionally confirmed by earlier works [93], showing that the valence of the B-cation, ionic radius, and ionic shifts exert a decisive

impact on T_C prediction. The component DCE_B describes the electron configuration of the B-cation, thus determining the covalence degree of the B–O bond. The expression $DCE_B \times V_B$ describes the relationship between the electronic configuration and geometric parameters of the atoms at the B-sites, where the atomic volume V_B correlates with the unit cell size and the free space left for ionic shifts. The expression $(DCE_B - DCE_A)$ represents the difference in the electron configurations of the B- and A-cations, caused by the distribution of electronic density and distortion of oxygen octahedrons. The latter descriptor covers the key factors determining the T_C of KNN-based ceramics: the electronic structure of the B-cation (DCE_B), lattice geometry (V_B), and balance of the electron configuration parameters of the A- and B-cations ($DCE_B - DCE_A$).

Conclusion

In this work, the prediction of d_{33} , ϵ , and T_C of KNN-based ferroelectric ceramics was carried out sequentially using a hybrid strategy, i.e., a combination of the Sure Independence Screening and Sparsifying Operator (SISSO) with ensemble machine learning methods (Extra Trees Regressor (ETR), Random Forest (RF), Gradient Boost-

ing Regressor (GBR), and eXtreme Gradient Boosting (XGBoost)).

For each target property (the piezoelectric coefficient d_{33} , the dielectric permittivity ϵ , and the Curie temperature T_C), descriptors were identified that exert the maximum impact on the predictive capability of the machine learning models. We showed that the best results in d_{33} prediction were achieved using the ETR model, delivering an average relative error of about 10.7 %. for the validation set which was not used for leaning. For ϵ , the smallest error (7.8 %) was also obtained for the ETR model, and for T_C , the best result was achieved using the RF model, the error being 6.7 %.

Thus, physically interpretable predictors were developed that allow accurate prediction of the key ferroelectric parameters of KNN-based ceramics. The results confirm the efficiency of the suggested approach combining the SISSO method with ensemble machine learning methods and open up new possibilities for the design of materials with tailored functional parameters.

Acknowledgments

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Supplementary information

Table 1S. Validation set for testing the target variable d_{33}

Sample number	Chemical formula
1	$0.959\text{K}_{0.48}\text{Na}_{0.52}\text{NbO}_3-0.04\text{Bi}_{0.5}\text{Na}_{0.5}\text{ZrO}_3-0.001\text{LaFeO}_3$
2	$(\text{K}_{0.465}\text{Na}_{0.465}\text{Li}_{0.07})\text{NbO}_3$
3	$0.958\text{K}_{0.48}\text{Na}_{0.52}\text{NbO}_3-0.04\text{Bi}_{0.5}\text{Na}_{0.5}\text{ZrO}_3-0.002\text{LaFeO}_3$
4	$0.97\text{K}_{0.48}\text{Na}_{0.56}\text{NbO}_3-0.03\text{Bi}_{0.5}\text{Li}_{0.5}\text{ZrO}_3$
5	$0.965(\text{K}_{0.5}\text{Na}_{0.5})(\text{Nb}_{0.96}\text{Sb}_{0.04})\text{O}_3-0.02(\text{Bi}_{0.5}\text{Na}_{0.5})(\text{Zr}_{0.8}\text{Ti}_{0.2})\text{O}_3-0.015\text{CaZrO}_3$
6	$(\text{K}_{0.44}\text{Na}_{0.52}\text{Li}_{0.04})_{0.99}\text{Cu}_{0.005}(\text{Nb}_{0.86}\text{Ta}_{0.10}\text{Sb}_{0.04})\text{O}_3$
7	$0.95(\text{K}_{0.48}\text{Na}_{0.52})\text{NbO}_3-0.05\text{Ca}_{0.15}(\text{Bi}_{0.5}\text{Na}_{0.5})_{0.85}\text{ZrO}_3$
8	$0.95(\text{K}_{0.48}\text{Na}_{0.52})\text{NbO}_3-0.05\text{Ca}_{0.4}(\text{Bi}_{0.5}\text{Na}_{0.5})_{0.6}\text{ZrO}_3$
9	$0.98(\text{K}_{0.5}\text{Na}_{0.5})_{0.94}\text{Li}_{0.06}(\text{Nb}_{0.96}\text{Sb}_{0.04})\text{O}_3-0.02(\text{Bi}_{0.5}\text{Na}_{0.5})(\text{Zr}_{0.8}\text{Sn}_{0.1}\text{Hf}_{0.1})\text{O}_3$
10	$0.96(\text{K}_{0.4}\text{Na}_{0.6})(\text{Nb}_{0.96}\text{Sb}_{0.04})\text{O}_3-0.04\text{Bi}_{0.5}\text{K}_{0.5}\text{Zr}_{0.6}\text{Sn}_{0.4}\text{O}_3$

Table 2S. Validation set for testing the target variable ϵ

Sample number	Chemical formula
1	$(\text{Na}_{0.5}\text{K}_{0.5})_{0.975}\text{Li}_{0.025}\text{Nb}_{0.74}\text{Sb}_{0.08}\text{Ta}_{0.18}\text{O}_3$
2	$0.96(\text{K}_{0.45}\text{Na}_{0.55})\text{NbO}_3-0.04\text{BaHfO}_3$
3	$0.95(\text{K}_{0.45}\text{Na}_{0.55})\text{NbO}_3-0.05\text{BaHfO}_3$
4	$0.94(\text{K}_{0.45}\text{Na}_{0.55})\text{NbO}_3-0.06\text{BaHfO}_3$
5	$0.95\text{K}_{0.5}\text{Na}_{0.5}\text{Nb}_{0.965}\text{Sb}_{0.035}\text{O}_3-0.01\text{CaSnO}_3-0.04\text{Bi}_{0.5}\text{K}_{0.5}\text{HfO}_3$
6	$0.96\text{K}_{0.5}\text{Na}_{0.5}\text{Nb}_{0.96}\text{Sb}_{0.04}\text{O}_3-0.01\text{CaSnO}_3-0.03\text{Bi}_{0.5}\text{K}_{0.5}\text{HfO}_3$
7	$0.96\text{K}_{0.5}\text{Na}_{0.5}\text{Nb}_{0.95}\text{Sb}_{0.05}\text{O}_3-0.01\text{CaSnO}_3-0.03\text{Bi}_{0.5}\text{K}_{0.5}\text{HfO}_3$
8	$0.96\text{K}_{0.5}\text{Na}_{0.5}\text{Nb}_{0.94}\text{Sb}_{0.06}\text{O}_3-0.01\text{CaSnO}_3-0.03\text{Bi}_{0.5}\text{K}_{0.5}\text{HfO}_3$
9	$0.96\text{K}_{0.5}\text{Na}_{0.5}\text{Nb}_{0.93}\text{Sb}_{0.07}\text{O}_3-0.01\text{CaSnO}_3-0.03\text{Bi}_{0.5}\text{K}_{0.5}\text{HfO}_3$
10	$0.98(\text{K}_{0.52}\text{Na}_{0.48})\text{Nb}_{0.95}\text{Sb}_{0.05}\text{O}_3-0.02\text{Bi}_{0.5}(\text{Na}_{0.8}\text{K}_{0.2})_{0.5}\text{ZrO}_3$

Table 3S. Validation set for testing the target variable T_C

Sample number	Chemical formula
1	$((\text{K}_{0.5}\text{Na}_{0.5})_{0.9506}\text{Bi}_{0.0194}\text{Li}_{0.03})(\text{Nb}_{0.9506}\text{Sc}_{0.0194}\text{Ta}_{0.03})\text{O}_3$
2	$0.95(\text{K}_{0.48}\text{Na}_{0.52})\text{NbO}_3-0.05\text{Ca}_{0.6}(\text{Bi}_{0.5}\text{Na}_{0.5})_{0.4}\text{ZrO}_3$
3	$0.96(\text{K}_{0.48}\text{Na}_{0.49}\text{Li}_{0.03})\text{NbO}_3-0.04\text{Bi}_{0.5}\text{Na}_{0.5}\text{ZrO}_3$
4	$0.96(\text{K}_{0.5}\text{Na}_{0.5})\text{NbO}_3-0.04(\text{Bi}_{0.5}\text{Na}_{0.5})\text{ZrO}_3$
5	$0.956\text{K}_{0.40}\text{Na}_{0.60}\text{NbO}_3-0.014\text{BiScO}_3-0.03\text{Bi}_{0.5}(\text{Na}_{0.6}\text{K}_{0.3}\text{Li}_{0.1})_{0.5}\text{HfO}_3$
6	$0.99\text{K}_{0.48}\text{Na}_{0.56}\text{NbO}_3-0.01\text{Bi}_{0.5}\text{Li}_{0.5}\text{ZrO}_3$
7	$0.956\text{K}_{0.48}\text{Na}_{0.52}\text{NbO}_3-0.04\text{Bi}_{0.5}\text{Na}_{0.5}\text{ZrO}_3-0.004\text{LaFeO}_3$
8	$0.956\text{K}_{0.48}\text{Na}_{0.52}\text{NbO}_3-0.04\text{Bi}_{0.5}\text{Na}_{0.5}\text{ZrO}_3-0.004\text{BiAlO}_3$
9	$0.96(\text{K}_{0.48}\text{Na}_{0.32}\text{Li}_{0.2})\text{NbO}_3-0.04\text{Bi}_{0.5}\text{Na}_{0.5}\text{ZrO}_3$
10	$0.959\text{K}_{0.48}\text{Na}_{0.52}\text{NbO}_3-0.04\text{Bi}_{0.5}\text{Na}_{0.5}\text{ZrO}_3-0.01\text{LaFeO}_3$